New Models and Numerical Codes for

Shock Wave Processes in Condensed Media

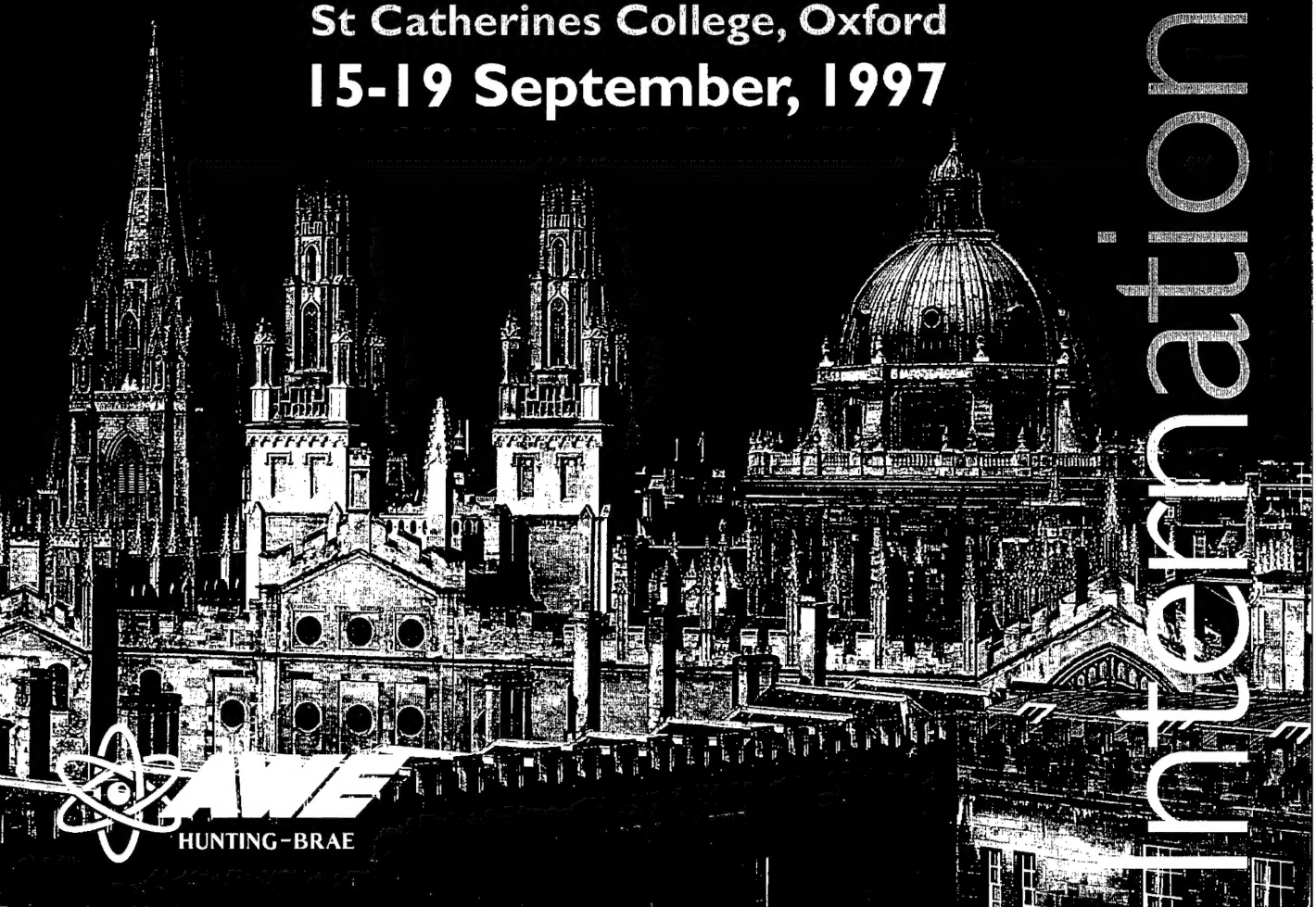
International workshop

Abstracts

(In presentation order & Poster sessions)

St Catherines College, Oxford

15-19 September, 1997



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HUNTING-BRAE

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on
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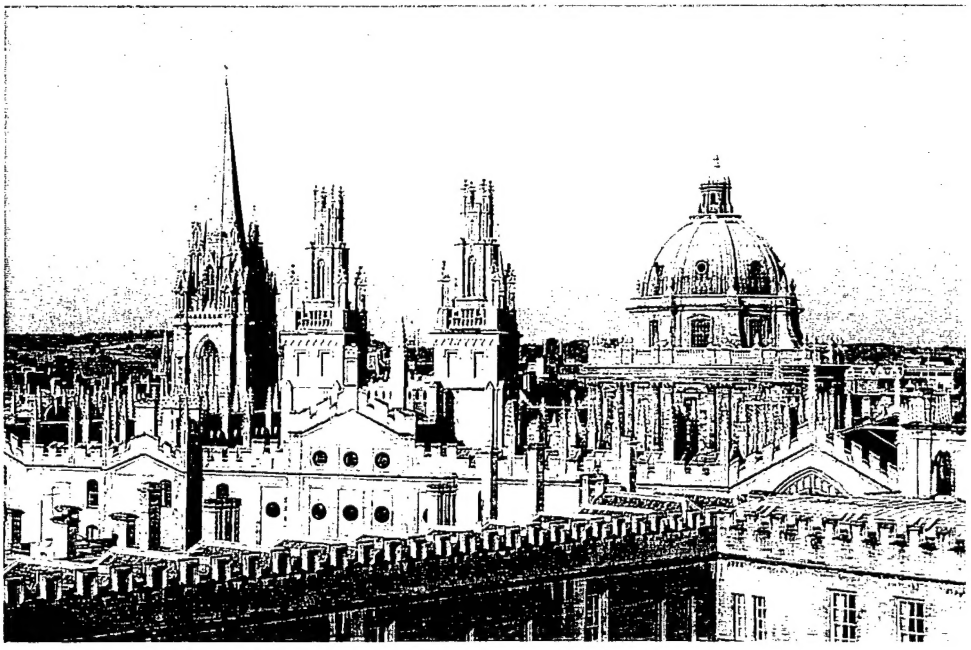

ABSTRACTS

(In Presentation Order + Poster Sessions)

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Acknowledgements:

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AWE Hunting Brae
UK Ministry of Defence
European Research Office, United States
Army Naval Research Office

PROGRAMME SUMMARY

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Sunday, 14 September

Registration Conference Office	1700 - 1900
Dinner at St Catherines (for residents) St Catherines	1930

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Monday, 15 September

Registration Conference Office	0830 - 0930
Conference Room A:	
Opening of Conference	0930
Technical Session: *New Hydrocode Development I*	0940
Technical Session: *Models of Detonation Processes I*	1400
Poster and Exhibition	1900 - 2100
Fork buffet	1930 - 2100

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Tuesday, 16 September

Conference Room A:	
Technical Session: *Numerical Schemes for Hydrocodes I*	0900
Technical Session: *Advances in Experimental Techniques 1*	1400
Conference Room B:	
Technical Session: *New Hydrocode Developments (SPH)*	1400
Dinner at St Catherines (for residents)	

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Wednesday, 17 September

Conference Room A:

Technical Session: *Models of Materials Under Shock Loading Compression*	0900

Conference Room B:

Technical Session: *Models of Detonation Processes II*	1050

Afternoon Free

Dinner at St Catherines *(for Russian delegates only)*	2000

Evening free*(non Russian delegates)*

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Thursday, 18 September

Conference Room A:

Technical Session: *Molecular Dynamics and Quantum Chemistry in Shock Waves*	0900
Technical Session: *Models of Ceramics Under Shock Compression II*	1110
Technical Session: *Equation of State of Hydrocodes*	1400

Conference Room B:

Technical Session: *Advances in Experimental Techniques II*	0900
Technical Session: *Numerical Schemes for Hydrocodes II*	1400
Banquet at St Edmund Hall	1900 for 1930

◇◇

Friday, 19 September

Conference Room A:

Technical Session: 0900
New Hydrocode Developments II

End of Workshop 1200

Lunch and Dinner at St Catherines for Russian delegates

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ABSTRACTS

A SURVEY OF NUMERICAL METHODS FOR SHOCK PHYSICS APPLICATIONS*

Eugene S Hertel, Jr

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Hydrocodes, or more accurately, shock physics analysis packages, have been widely used in the United States Department of Energy (DOE) laboratories and elsewhere around the world for over 30 years. Initial applications focused on weapons effects where the pressure levels were high enough (substantially above the yield surface of representative materials) to disregard the material strength, hence the term "hydrocode". Over the last 30 years, Sandia has worked extensively to develop and apply advanced hydrocodes to armor/anti-armor interactions, warhead design, high explosive initiation, and weapon safety issues. The needs of the DOE have changed over the last 30 years, especially over the last decade. A much stronger emphasis is currently placed on the details of material deformation and high explosive initiation Phenomena. The hydrocodes of 30 years ago are now sophisticated analysis tools that can replace testing in some situations and complement it in all situations.

A brief history of the development of hydrocodes at Sandia will be given. The emphasis will be on the development of our current multi-dimensional code, CTH. CTH is a family of codes developed at Sandia National Laboratories for modelling complex multi-dimensional, multi-material problems that are characterised by large deformations and/or strong shocks. A two-step, second-order accurate Eulerian solution algorithm is used to solve the mass, momentum, and energy conservation equations. CTH includes models for material strength, fracture, porosity, and high explosive detonation and initiation. The Johnson-Cook, Zerilli-Armstrong, and Steinberg-Guinan-Lund material models are available within CTH. These models rely on the use of internal state variables (typically the equivalent plastic strain) to account for the history dependence of material response.

I will also discuss and compare the four principal methods in use today for the solution of the conservation equations of mass, momentum, and energy for shock physics applications. The techniques discussed are the Eulerian methods currently employed by CTH; the element based Lagrangian method currently used by codes like DYNA; the element free Lagrangian method (also know as smooth particle hydrodynamics) used by codes like SPHINX; and the Arbitrary Lagrangian Eulerian methods used by codes like CALE. The numerical subtleties of these techniques will be discussed and example simulations will be provided.

* This work performed at Sandia National Laboratories supported by the US Department of Energy under contract number DE-AC04-94AL85000.

RUSS-2DE HYDROCODE WITH THE TVD PROCEDURE

G S Romanov, A E Suvorov, I M Kozlov, V Yu Klimenko*

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*High Pressure SIC, Institute of Chemical Physics, Moscow, Russia

The RUSS-2DE [1] is a two-dimensional, explicit, finite-difference Eulerian hydrocode for simulations of the shock wave processes in high explosives, metals and plastics. It operates in plane and cylindrical geometry.

The hydrocode employs the TVD procedure based on the predictor-corrector method of the second order of accuracy with respect to time and space. Although we use a high-accuracy numerical scheme, we do not obtain the mathematical oscillations behind the shock wave front, because the TVD procedure [2] permits to maintain the steep gradients without introducing the non-physical oscillations. Two perfect interface tracking method is applied for description of material interfaces.

The Multiprocess model of detonation [3] is used for simulation of the explosive reaction to shock wave action. The elastic-plastic model describes the plastic deformation of materials. The viscoelastic Maxwell-like body model [4] is applied for description of intense dynamic deformations in metals.

A high-level graphs for clear representation of the results both during and after computation and favourable interface maximally simplifies the work of a user with the RUSS-2DE hydrocode.

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SHAMROCK - AN ADAPTIVE, MULTI-MATERIAL HYDROCODE

Brian J Jones

AWE Aldermaston, UK

A description will be given of a new hydrocode that couples a staggered mesh, Lagrange/remap method with a block patching dynamic mesh adaptation met hod (Quirk 1991).

The Choice of a staggered mesh algorithm greatly simplifies the inclusion of a constitutive strength model. Currently implemented is an elastic-viscoplastic model developed at AWE (Gray 19??).

Material interfaces are reconstructed using the technique developed by Youngs (Youngs 19??). At the present time, all interfaces are held at the highest level of refinement, but it is expected that the block patching approach to adaptation will allow for less critical interfaces to be relaxed to lower resolution in the near future.

The code may run either with (i) temporal refinement where less refined computational cells are advanced less often with larger timesteps or (ii) in a mode where all cells are advanced with the same timestep but with the ability to automatically and robustly restart a calculational step with a reduced timestep in the event of a user specified accuracy condition being exceeded.

The code has been linked to a comprehensive in-house equation of state library and now benefits from an ignition and growth high explosive detonation package (Whitworth 1995) and an implicit material spall model (Giles 1995). The paper will pay particular attention to the following:

Choice of numerical scheme and adaptation methodology.
Adaptation Criteria.
Code Structure.
Results illustrating the benefits of the approach.

NUMERICAL SIMULATION OF DETONATION IN CONDENSED PHASE EXPLOSIVES

David A Jones

Aeronautical and Maritime Research Laboratories, Melbourne, Australia

The development of a two-dimensional multimaterial Eulerian hydrocode to model the effects of detonating condensed phase explosives on surrounding materials is described. The code solves coupled equations for the conservation of mass, momentum, and energy for an inviscid compressible fluid. Operator splitting is used to reduce the complexity of the two-dimensional calculation and the resulting one-dimensional equations are solved using the Flux Corrected Transport (FCT) algorithm of Boris and Book. Ideal explosives are described using either the BKW Equation of State and Forest Fire reaction rate model or the JWL EOS and the Ignition and Growth model. Highly non-ideal underwater explosives are described using a polytropic EOS with a density dependent index, and the associated reaction rate is based on a three term model originally derived for composite porous explosives. The Mie-Gruneisen EOS is used to describe non-energetic materials.

Two interface tracking algorithms to maintain a sharp interface between different materials on the computational mesh have been implemented and tested, and two different transport schemes have been tried. The first approach uses the Simple Line Interface Calculation (SLIC) of Noh and Woodward with an additional modification to account for corners. In this scheme the individual material densities are resolved and transported independently, but only the total energy and momentum in a mixed cell are transported, hence an iterative procedure is then required to determine the internal energy of each material in a cell. An alternative scheme uses a modified Youngs interface tracker and a transport algorithm in which both the individual material densities and specific energies are convected. This removes the need for a time consuming iteration on the internal energies in a mixed cell. The advantages and disadvantages of both approaches will be described.

Several applications of the code to recent problems will then be described. These include the use of the code to simulate the impact of cylindrical steel projectiles against explosives. The code has been used to determine the threshold velocity for the onset of detonation as a function of projectile diameter and the computed results are in good agreement with experimental values, as well as with

results obtained from other reactive codes. Other applications include one and two-dimensional underwater explosives effects simulations.

TREK HYDROCODE FOR NUMERICAL SIMULATIONS OF 3-D FLOWS OF MULTICOMPONENT MEDIUM

Yu V Yanilkin, V I Tarasov, A I Stadnik, S V Bazhenov, V V Bashurov,
S P Belyaev, Yu A Bondarenko, E S Gavrilova, V V Gorev, 0 Dibirov,
G G Ivanova, N P Kovalev, T V Korol'kova, P 1 Pevnaya, A A Shanin,
V N Sofronov, T A Toropova

Russian Federal Nuclear Center - VNIIEF, Arzamas-16, Russia

The report is devoted to description of multi-purpose TREK hydrocode, intended to numerical simulation of 3-D flows of multicomponent medium characterised by large deformations of interface boundaries.

The report considers the most general ideas and principles, laid into the groundwork of hydrocode organisation, and discusses the methods for solving the problem of initial data calculation and visualisation of calculation results.

The hydrocode is intended for numerical simulation of gasdynamic flows with regard to strength of materials, diffusion processes, detonation of explosives, turbulent mixing and poly-disperse medium flows. Approximation for the differential equations is produced in Eulerian or Lagrangian-Eulerian variables. The concentration method is used for interface boundaries calculation, making possible to localise the boundaries with an accuracy of one calculating cell. The brief description of calculating modules implemented within the hydrocode is adduced.

There are presented the examples of simulation of some tasks by the TREK hydrocode: the evolution of thin shell perturbations; the impact penetration; the rising up of explosive cloud; the aerosols transport in atmosphere, et al. The calculation results are compared with the experimental data and with the results of calculations by the other methods. We have got a good agreement.

DEVELOPMENT OF CALCULATION TECHNIQUE FOR CONNECTIVE FLOWS AND ITS IMPLEMENTATION IN MIMOZA HYDROCODE

V V Zmushko

Russian Federal Nuclear Center - VNIIEF, Arzamas-16, Russia

The MIMOZA hydrocode was designed for the ELBRUS-2 computer in the mathematical section of the VNIIEF Center at the end of the 80-s. The hydrocode is intended to solve multidimensional problems in continua mechanics, 2-D and 3-D problems in gas dynamics with heat conductivity.

The hydrocode is based on principles realised earlier and successfully verified.

ERROR ESTIMATION FOR HIGH-VELOCITY DYNAMIC PROBLEMS

J P Combe* - P Coorevits* - A Fanget** - J P Pelle*

*Laboratoire de Mechanique et Technologie, ENS de Cachan/CNRS/UPMC
**Centre d'Etude de Gramat

Numerical simulations of high-velocity impact problems are performed using explicit programs. Moreover, these simulations require taking into account non-linear constitutive laws, large strains, as well as contact laws between projectile and target. Simulations resulting from such kinds of problem are most difficult to control. The aim of the present study, which is a collaborative effort between the LMT Cachan and the CEG, is both to develop error measures able to evaluate the discretisation errors, and to define remeshing procedures that allow computing high-quality dynamic simulations.

Built on *a posteriors* estimators, which are based on the notion of "error in the constitutive relation" and which have been developed at Cachan for many years ' an error measure for linear dynamic problems is proposed herein. This estimator is composed of two terms, one referring to strain energy and the other to kinetic energy, and allows evaluating errors linked to both time and space discretisations.

It was initially computed for explicit unidimensional dynamic problems. Results obtained from tests where analytical solutions are known, show that the proposed measure provides an accurate estimation of the actual error. Moreover, its estimation quality is enhanced as the time step approaches that associated with the CFL stability condition.

Afterwards, this error estimator algorithm has been programmed for explicit bidimensional dynamic problems, and a simple, time-dependent remeshing procedure has been defined. Numerical results obtained on simple structures will be presented.

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[2] P Coorevits, P Ladeveze, J P Pelle, *Anisotropic adaptive mesh: Application to transient problems,* Proc of the First European Conference on Numerical Methods in Engineering, pp 209-215, BRUXELLES, 1992 [3] P Coorevits, P Ladeveze, J P Pelle, *An automatic procedure for finite element analysis in 2D elasticity, Computer Methods in Applied Mechanics and Engineering, Vol 121, pp 91-120,* 1995

AN OVERVIEW OF NUMERICAL DETONATION MODELS

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High Pressure SIC, Institute of Chemical Physics, Moscow, Russia

Impetuous progress in computer technique changes qualitatively the situation in shock wave science. In the 60-80 years the experiment dominated in our investigations. However, already now the computer simulation becomes a powerful toot in the study of shock wave phenomena. The numerical experiment (instead of the real physical experiment) gives possibility to discover the interior deep mechanisms of explosion processes, which are inaccessible for the existing experimental technique.

For example, the pore collapse in explosive under shock compression and the creation of the hot spot is a very complex process. The pore is very small (- 1 gm), the time duration of the process is also small (~ 0. 1 μs), and the explosive is opaque. Clearly that any experiment can not indicate in detail this process. But, the computersimulation [1] permitted to discover and to analyse the physical nature of the porecollapse comprehensively. Or another example, the explosive initiation by theprojectile is very important for practice. But, until now the physical mechanism of theinitiation process in critical conditions was not studied. Many years many researchers studied this process experimentally and theoretically and established some criterions of initiation, but the interior physical nature was not determined. Only recently the careful numerical simulations [21 gave the detailed information about the mechanism of this very complex process.

However, the computer simulations will be most important and successful for applied developments, for the design of new engineering systems.

Therefore, by 2000-2002 years we shall have the supercomputers with performance 10-100 Teraflops. It means that at last we receive a possibility to simulate physical processes in explosives, metals with great resolution (ie to use the fine numerical grid). If, for example, we apply the adaptive gridding procedure with the mesh size from 0.01 mm to 1 mm than we can simulate the real engineering systems (size = 10-00 cm) and use the fine zoning (- 0.01 mm) for most important computational regions (shock fronts, interfaces, large gradients in some physical parameters).

In this case (the mesh size - 0.01 mm) we can simulate the real reaction zone *for* detonation process and use the perfect physical models of detonation with high accuracy. So, it is not necessary to apply the empirical (not physical, but mathematical - approximated) detonation models (for example, the very famous WBL [31 and DSD [4] models) for such calculation, because these models have more low accuracy and can not simulate exactly the complex detonation processes (for example, the shock-to-detonation transition). Before the preparation of the physically perfect model it is necessary to analyse the existing models and to outline the strategy for such activity.

This report presents the overview and the analysis of the existing numerical models of detonation that are constructed on the bases of physical processes occurring in explosive during detonation.

In the first part we give the overview of the physical mechanisms that are discovered by now. This is the hot-spot mechanism, ie the collapse of the pore in explosive, the viscoplastic heating of the explosive layer around the pore and decomposition of this heated explosive. At the beginning the mechanism was studied in some classical investigations [5-71, but most successful and comprehensive consideration is given in the work [1). We also discuss the frontal mechanism that was first proposed in 1980 [8] and developed in the next papers (for example, [9]). The mechanism has two stages (intra-frontal and post-frontal). The intra-frontal stage proceeds in a shock wave front and its governing process is the temperature overheating. Radicals are generated at this stage. At the second stage they activate a some set of consecutive parallel reactions that results in final products with corresponding energy release. At last we consider the dislocation mechanism [10]. The high speed dislocations (responsible for high rate plastic deformation) generate phonons of sufficient energy for resonant excitation of the vibrational modes of explosive molecule. This exited molecules decompose and activate the later decomposition of the surrounding explosive. All these mechanisms act together, ie in parallel regime. But, the hot spot mechanism dominates in the low pressure region and the frontal mechanism - in the high pressure region. This multiprocess idea was first proposed in 1988 (11)

In the second part we give the overview and the analysis of the most famous numerical models of detonation. At the first we consider the hot spot models: the ignition and Growth model [12, 13], the Explicit Hot Spot model [14], the Kim's model [151 and the AMORC model [16]. At the second we discuss the Multiprocess model [9]. And at the last we analyse the predictive performance of the

discussed models and consider the possibility for preparation of the physically perfect model of detonation.

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THEORETICAL AND COMPUTER MODELS OF DETONATION IN SOLID EXPLOSIVES

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Recent experimental and theoretical advances in energy transfer and chemical kinetics have led to improved descriptions of detonation waves in solid explosives in both the theoretical Nonequilibrium Zeldovich-von Neumann- Doring (NEZND) model and in computer reactive flow models. Picosecond laser excitation experiments and molecular dynamics modelling have measured the phonon up-pumping and internal vibrational energy redistribution (IVR) rates at which the unreacted explosive molecules are excited to the transition state that leads to chemical reaction behind the leading shock front. Laser interferometry has been used to determine the induction time for chemical reaction at the von Neumann spike state. Once the exothermic chain reactions begin, the reaction products are formed in highly excited vibrational states, which equilibrate rapidly via supercollisions that transfer several quanta of energy in one collision. Embedded gauges and Fabry-Perot techniques are used to measure the rates at which these reaction products expand and thermally and chemically equilibrate. In carbon-rich solid explosives, the relatively slow formation of large carbon particles of diamond or graphite extends the overall reaction zone length and leads to lower Chapman-Jouguet (CJ) pressures that previously used.

To better simulate these chemical kinetic processes, completely temperature dependent reactive flow modules are being developed in the ALE3D hydrodynamic code. In some situations, these models yield better simulations than the compression and pressure dependent Ignition and Growth reaction flow model, which has calculated many 1 D, 2D and 3D shock initiation and detonation flows for over 15 years.

EQUATIONS OF STATE OF TWO-PHASE REACTIVE MIXTURES FOR APPLICATION TO EXPLOSIVE INITIATION MODELLING IN CONJUNCTION WITH FRONT-TRACKING

Dr John Starkenberg

US Army Research Laboratory Aberdeen Proving Ground, USA

We are planning to adapt a front-tracking "hydrocode" developed at the State University of New York at Stony Brook for application to solid explosive initiation problems.

The principal elements required to treat such problems numerically are a continuum mechanics model (including appropriate treatment of boundary conditions) and a reacting mixture model. The former is represented by a system of dynamic partial differential equations and the latter by a system of algebraic equations (augmented, in some cases, by additional dynamic equations). The forms of the these models depend on the assumptions used.

The front-tracking code is unique in that it limits solution of the dynamic continuum mechanics equations to regions bounded by tracked fronts. It uses local solutions of the Riemann problem to advance the positions of tracked shock waves and contact discontinuities. This places stringent requirements on the availability of thermodynamic information.

In order to limit the amount of work required to adapt the code, we are interested in mixture models that, insofar as possible, allow retention of the gas dynamics conservation equations for diffusionless flow. The extent to which this objective may be achieved depends on the physical assumptions that we wish to apply. Usually, this requirement can be met, although additional dynamic equations may arise. It is generally necessary to add a dynamic equation representing reaction progress.

Several modelling approaches applicable to mixtures of discrete phases have been reported in the literature and some of these are reviewed and amplified here. In general, they are based on known equations of state for each phase.

The set of physical assumptions that appears to best apply to explosive initiation includes mechanical equilibrium and thermal isolation between reactant and product phases. While the thermal isolation condition can be implemented as an added dynamic equation, representing partitioning of the energy conservation equation between the phases, including it directly in the mixture model is more consistent with our desire to retain the original form of the conservation equations. We have developed a model along these lines that can be used independent of the choice of equations of state for the phases. This model depends on a reference state defining the reactant isentrope and requires dynamic advection of the associated state variables. Using the resulting equation of state, we have developed expressions for the thermodynamic functions required by the front-tracking code. These include the mixture pressure, sound speed, Grueneisen function, temperature, and specific heat. In addition, isentrope and Hugoniot functions have been determined.

DEVELOPMENT OF HOT-SPOT MODEL FOR EXPLOSIVE DECOMPOSITION IN WEAK SHOCK WAVES

S G Andreev

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A model developing Eyring, Powell and Duffey approach is presented. This model uses an integration of approximate analytical solutions obtained from the analysis of a number of heuristic models for some processes and regularities which were detected in special experiments (an investigation of explosive decomposition at homobaric conditions produced by weak shock waves). The system of formal kinetic equations is derived. It is used for study of the influence of the burning law, the pore gas compressibility and the grains size distribution of matrix substance and pores on the shock sensitivity of explosive charges. The decomposition rate is presented by the product of three components. The first component describes the change of area of laminar burning surface for the hot spots (with spherical or cylindrical shape) generated by visco-plastic collapse of spherical or cylindrical pores. The second component describes the laminar burning in quasistatical approximation. In this case it is possible to set the limits for the pressure decrease rate resulted in the explosive extinction. The third component named correction component, in general case, is the product of two functions that decrease rapidly with increase of decomposition degree and time (similarly to the first term in the Tarver's "ignition and growth" model. The first function accounts for the influence of inhomogeneous heating of porous explosives at shock wave compression. The second function takes into account the stream mechanism for distortion of spherical or cylindrical shape of initial hot spots.

The simplest version of the formal kinetics equations (explosive grains are of the same size, explosive is deformed by reaction products without the breakdown of entirely along the grain boundaries) was used for numerical simulations. An evolution of shock waves in explosive charge under the impact of plates of different thickness was studied. Possibility of anomalous increase of

the detonation delay near the critical conditions of initiation was indicated. Analysis of the computational and experimental data has led to the assumption that it is necessary to take into account the presence of fine-grained fractions in explosive and the stream mechanism of burning propagation for adequate description of the decomposition at the beginning of its progressive stage.

INITIATION BY IMPACT OF SHOCK

Charles S Coffey

Indian Head Division, Naval Surface Warfare Center, Indian Head, USA

This paper presents some recent advances in the initiation of explosives by impact. These first principal calculations examine initiation due to the energy dissipated during plastic deformation of the explosive crystals by the impact or shock. Several experiments situations are considered including the drop weight impact test, a large calibre gun setback simulator and a porous bed DDT test. Predictions of the initiation impact levels and behaviour are made and compared with the experimental data. Since the theory treats both shock and impact initiation it is able to provide a useful link between these stimuli. This will be illustrated in the case of DDT in a porous bed of HMX. The link between impact and shock initiation will also be shown to account for the ability of the small scale Ballistic Impact Chamber Test to rank the relative shock initiation sensitivity of explosives. An outcome of this work is the ability to treat impact and shock initiation in a unified way.

DISLOCATION MECHANICS ASPECTS OF DEFORMATION-INDUCEDDETONATIONS AND DYNAMIC DEFORMATIONS

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*University of Maryland, College Park, USA; +Loyola College, Baltimore, USA; #Potomac,USA;
**Naval Surface Warfare Center-IHD, Indian Head, USA

Model dislocation pile-up calculations have supported a "hot spot" explanation of larger drop weight heights required for initiation of smaller sized energetic crystals in impact sensitivity tests [1]. Theoretical stress concentrations for cleavage fracturing and consequent viscoplastic slip band avalanches are key elements of the dislocation mechanics based description. These features are relevant [21 to the initiation of detonation in that they connect fundamentally with the molecular bonding of energetic crystal lattices that are, in general, relatively brittle despite being elastically compliant. Intermolecular blockages of dislocation motion by adjacent out-cropping molecular appendages account for the low ductility/brittleness properties. The desired situation is opposite for most structural metals and alloys normally experiencing the brunt of high deformation rates from energetic material detonations. However, when subjected to high rate loading conditions, metallic alloys also show increasingly difficult viscoplastic deformations and plastic instability behaviours that are accounted for with analogous dislocation mechanics based constitutive equations [31. The equations distinguish, for example, between body-centered cubic and relatively more ductile face-centered cubic materials. Under high stress amplitude shock loading conditions, additional dislocation generation and deformation twinning mechanisms come into operation to further complicate material behaviour. The method of molecular dynamics is well suited to deciphering these behaviours under such conditions, both for validating the "hot spot" character of plastic relaxation at the molecular scale and for elucidating mechanisms of dislocation generation at manoscale dimensions [4].

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DETONATION WAVE PROPAGATION IN CONDENSED EXPLOSIVES ACCORDING TO THE RELAXED JOUGUET MODEL

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Two directions are currently used to solve the detonation wave propagation problem. The first one considers the detonation front as an inert, downstream subsonic shock behind which the chemical reactions being. This is a totally kinetic method. The second direction assumes the front to be completely reactive and self-sustained (downstream sonic). the front can be propagated independently of downstream conditions. This is a non kinetic method. A new model which combines both aspects describes the detonation wave propagation in condensed explosives; the so called relaxed Jouguet model (Jr), has been proposed by L Brun.

According to the Jouguet model, the infinitely thin, downstream sonic and totally reactive detonation front has a constant velocity. The Jr model keeps the assumption of downstream sonicity but does not suppose, as Jouguet did, a total decomposition within the front. The detonation does not propagate with a constant velocity and its acceleration is directly related to two characteristic functions of the explosive. The first one is the classical curvature vs. detonation velocity function. The second one is a new function: front waves velocity vs. detonation velocity. It describes how information propagates along the detonation front. Finally, a third characteristic function provides the limit condition at the interface between the detonation front and the confinement. This is the edge detonation angle vs. edge detonation velocity function.

In this paper, we briefly present a comparison between the detonation propagation methods. Then we recall the different assumptions of the relaxed Jouguet model and describe experiments performed to measure the three characteristic functions in a TATB - based composition. Finally, we compare, in a bidimensional plane case, chronometries and front profiles obtained numerically according to the JR model or to Huygens method with experimental profiles.

CAVITATIONAL MECHANISM OF DETONATION DECOMPOSITION IN LIQUID EXPLOSIVES

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It is accepted to consider that the mechanism of liquid explosive decomposition has character of homogeneous thermal explosion. However the minor dilution of these explosives with some liquids

(for example, an acetone) changes essentially a picture of detonation of homogeneous explosive systems. The pulsing regime of detonation arises and the significant part of explosive does not decompose.

In the present study the pulsing regime is considered from point of view of cavitational mechanism because frequency and intensity of the power field in the chemical reaction zone correspond to the conditions of cavitation.

Phenomena accompanying the cavitation process explain all conditions of the pulsing detonation for mixture (nitromethane + acetone) - overheating in some points of the liquid explosive, redistribution of the component concentration in the liquid mixture (concentration of explosive increases in the cavitation zone and decreases in the rest part of the mixture).

Only in the zone of cavitation where liquid explosive has increased concentration the decomposition of explosive takes place in the regime of overcompression as a result of cavitational pore collapse. The chemical reaction does not proceed apart from the cavitation zone. Shock wave front initiates the decomposition reaction only through formation of the cavitation zones.

The cavitation phenomenon takes place also in nondiluted liquid explosive. In this case the diluent with low temperature of boiling is absent and the power field has probably more high frequency. Therefore cavitation centres are more small and practically coalesce with each other forming the homogeneous region.

CHARME: A NEW PHYSICAL (BUT SIMPLE) REACTION-RATE MODEL FOR PRESSED EXPLOSIVES

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Shock to detonation transition of explosives is now widely thought to be due to hot spots. But the mechanism which causes the localisation of energy is still discussed. A lot of possible mechanisms have been proposed including shear bands, compression of trapped gases in pores, viscoplastic collapse of pores or friction between the two lips of a crack. It is likely that all these mechanisms can contribute depending on the conditions. A physical and rather complex model has been recently developed to simulate the ignition of pressed explosives (Saurel et al, 1997, to be published). There, shock to detonation transition is thought to result from hot spots created by the viscoplastic collapse of pores. The process is completely modelled with its mechanical, thermal and chemical aspects. This model was developed with a special ID hydrocode and a special numerical scheme and it seems to be a very hard task to extend it to multidimensional geometries. This model has then been used to build a simplified one (CHARME) which has been included in an existing eulerian-lagrangian hydrocode. The new model takes into account results of induction times and minimum radii of pores excited by a given shock pressure to compute the reaction rates. These data were calculated with the previous physical model and were tabulated. Ignition is modelled as a combustion by parallel layers inside the pores following an induction time. Then, after a moment, a transition pore - grain happens and grains begin to burn. The number of necessary parameters is limited and all of them have a clear physical meaning. Using the distributions of pores and grains as parameters instead of a unique size allows to assess the effects of these distributions on sensitivity of explosives. For instance, the so-called sensitivity reversal effect was successfully reproduced. Simulations of 1 D and 2D experiments with pressed HMX have been conducted. Data of simple and double plane shocks were fairly simulated. Ignition thresholds for impacts by rods with various diameters were determined and successfully compared to our experiments.

ARBITRARY LAGRANGIAN-EULERIAN HYDRODYNAMIC CALCULATIONS IN TWO DIMENSIONAL AT LLNL

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The arbitrary Lagrangian-Eulerian (ALE) hydrodynamic method tries to combine the efficient computational grid of Lagrangian methods with the robust character of Eulerian methods. ALE calculations in two dimensions have been used at LLNL since 1975 to successfully calculate a wide variety of difficult problems. A brief description of the ALE method is given and the results for several ALE calculations are presented.

ALE in CORVUS

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The paper describes the Arbitrary Lagrangian Eulerian (ALE) package which has been developed for the 2D Lagrangian hydrocode CORVUS. The algorithm is described along with details of the CORVUS implementation. CORVUS ALE employs the interface reconstruction method developed at LLNL for CALE and builds upon the existing SALE package in CORVUS.

The ALE package has been validated on a series of idealised test problems on both the Cray C98D and IBM SP2 super computers, the results from these calculations are presented. The ALE package has also been applied to a range of real problems of interest to AWE. These problems will be presented and comparisons drawn with available experimental data, pure Lagrangian and Eulerian calculations. A discussion is included of the potential benefits of using the CORVUS ALE method over pure Lagrangian and Eulerian codes at AWE is given and recommendations are made of how to best use the ALE method. The paper concludes with recommendations for future work.

EXTENSION OF LAGRANGIAN METHODS TO UNEQUAL ANGLE AND HIGHLY DISTORTED GRIDS

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In this work we present results that extend the range of applicability of Lagrangian numerical methods in two different but synergistically related ways that demonstrate a qualitative improvement in simulation capability. First, we show how Lagrangian algorithms can be changed in a very simple way that allows cylindrical and spherical symmetry to be preserved in cartesian and cylindrical geometry, respectively, for unequal angle zoning. This is done not only for the traditional area-weighted schemes that preserve this property only for equal angle zoning, but also in cylindrical geometry for the true control volume scheme that is more natural for constructing difference equations. This is effected by modifying the gradient operator that acts on the zone pressure in an automatic way that changes the zone edge lengths slightly so that when these symmetrics are present in the pressure field and boundary conditions of a physical problem the numerical scheme will also yield this symmetry. This allows not only a wider range of setups but removes the sensitivity of the calculations for applied perturbations that deviate from this symmetry. On problems without

the aforementioned symmetries we show that the modified gradient operator produces very little change in the results relative to the unmodified form.

The second thrust of this work is to extend the Lagrangian assumption to include the nodal mass on a staggered grid. This not only eliminates momentum flux of a node but "implies" the existence of subzonal Lagrangian corner masses. This in turn impliessubzonal pressures. A suitable discretization of these pressures is given and it is shown that hourglass and spurious vorticity motions that have been the bane of these methods can be eliminated. This allows the computation of smooth flows on grids that are highly distorted initially. All grid tangling can be eliminated with the proper specification of a single parameter that is easy to choose. There does remain the problem of ascertaining that the code, while still running, might give incorrect results. For some extreme cases it can be shown that the grid will bind unphysically. This difficulty will be discussed. The results mentioned will be documented with a wide variety of numerical examples, each interrelated and chosen to illustrate and justify the claims made above.

CALCULATIONAL TECHNIQUE FOR SHOCK WAVES WITH ELEVATED MONOTONOCITY

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In many difference techniques which are used for shock wave calculations the quantities profiles in the vicinity of shock layer which substitutes the strong discontinuity are non-monotonic. In a number of techniques [1] non-monotonicity is conditional and the oscillations amplitude could be minimized by selection of receptive Cuorant number. There are absolutely non-monotonic [2] and absolutely monotonic [3] techniques. The property of last one is that the decreasing the Courant number the discontinuity is strongly "spreaded".

The oscillations and the discontinuity "spreading" are initially the calculational phenomena. Their influence on the processes taking place in a substance after the shock passing have not been studied sufficiently. Various processes such as phase transfer, chemical reactions, destruction, etc could be initiated behind the shock front. The qualitative influence of the oscillations and the profile "spreading" on evolution of mentioned processes is considered here for some of model problems. The substance is "deceived" concerning the true conditions under which it is and its behaviour is incorrect. The dependence of destruction point co-ordinates and new phase origin versus the oscillation amplitude or the gap "spreading" width.

To minimize the mentioned effects the calculational technique for discontinue solutions of fluids dynamics is proposed in the present work. The property of profile monotonicity is combined with minimization of the gap "spreading" width. This result is achieved by application of special form of difference equations and Hugoniot equations for description of energy dissipation in the "spreading" zone. The results of the calculations of a number of standard problems (shock waves, rarefaction waves) are given.

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ON NEW RIEMANN SOLVERS FOR SHOCK HYDRODYNAMICS

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Godunov methods are becoming the established numerical technology to model shock wave phenomena in various media, eg gases, liquids and solids [21. A Godunov method requires the solution of local Riemann problems. For general materials there is ample justification for solving the Riemann problem approximately. However, the quality of the Godunov numerical technology depends crucially on the quality of the approximation to the solution of the Riemann problem.

In this paper, we first review conventional Riemann solvers and highlight their shortcomings for range of shock wave phenomena in single and multiphase shocked flows. We then present two classes of Riemann solvers for gaseous media. The first class provides an approximate state from which an intercell Godunov flux may be computed. The second class gives an intercell flux directly and is an extension of the Harten- Lax-van Leer (HLL) approach [11. The HLL approach assumes a twowave pattern in the solution of the Riemann problem. As a consequence, contact/ material interfaces and shear waves are smeared to unacceptable levels. Such smearing has in turn a large effect on the rest of the flow when complex wave interaction takes place. We then present the HLLC Riemann solver. This is formulated for general three dimensional systems. In this Riemann solver the missing waves in the HLL solver are restored. Numerical examples to illustrate the improvement of the HLLC over the HLL are given. The two classes of Riemann solvers are then extended for materials with general equation of state. Applications are shown for shocked flows in single and multiphase media.

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EGAK-EP METHOD FOR CALCULATIONS OF FRACTURE AND FRAGMENTATION OF MATERIALS

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The report presents the Lagrangian-Eulerian elastic-plastic EGAK-EP method implemented into the EGAK hydrocode [1]. The method is intended for 2-D flows simulations of multicomponent mediums characterized by large deformations. The concentration method is used for calculation of the interface boundaries.

Both the simple models based on the immediate destruction when achieving critical extended tensions and more complicated models are used for substance fracture calculations. The latter models include the equations for the parameters characterizing the degree of porosity of substance.

Declarations developed in works of Grady [2], Ivanov et al [3] are used for calculation of destroyed substance fragmentation process.

There are adduced the calculation results for soon problems: penetration of the two-layer (aluminium and textolit) target by the steel sphere; mutual impact of two copper plates; penetration of the plastic target by the steel sphere and so on. The methods for calculation of fragmentation have been tested on the last problem.

The calculation results are compared with the analytical solutions, the experimental data and the results of calculations by the other methods. There was obtained a good agreement for the calculation results with the analytical solutions and the experimental data.

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SHOCK-CAPTURING SCHEMES ON MOVING ADAPTIVE MESHES

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An efficient method for solving the Euler and Navier-Stokes equations for a numerical simulation of processes with shock waves by means of shock-capturing schemes on adaptive moving meshes.

A numerical method is proposed to generate a dynamic adaptive mesh. Meshes are adapted to the domains, where the physical solution has severe solutions. There is no need to interpolate the solution from the mesh at one time step to the next since the moving system of co-ordinates is used. In the Computational domain the mesh is uniform and fixed. A variational problem is solved to generate the mesh at each time step and an efficient numerical method is proposed to solve the problem. The efficiency is demonstrated by examples of one-dimensional test problems and the 3D explosion of a meteorite into the atmosphere. The Euler and Navie-Stokes equations are solved using the second-order UNO scheme and the third-order compact scheme.

The grid generation method is based on the minimization of a functional which includes measures of an adaptation to the solution, orthogonality and smoothness. The above technique was tested for a number of 1 D, 2D and 3D problems and explicit and implicit difference schemes.

THE IMPORTANCE OF PSEUDO-VISCOSITY IN THE DETERMINATION OF TEMPERATURE IN HYDROCODE SIMULATIONS

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Hydrocode simulations for the study of detonics, penetration mechanics and generalised shock processes in condensed matter are well established. With the pressures on R&D budgets and restrictions on the ability to perform full scale experiments, there is an increasing requirement for hydrocode simulations to replace many experimental measurements.

The philosophy adopted seeks to use hydrocode simulations to predict scaled experiments and the experiments to modify the code. The code is then used to design the rest of the system and guide experiments to crucial design features and performance parameters. Success within this cycle then implies the ability to simulate the full scale experiments.

Fundamental to this philosophy is the ability to accurately predict material deformation at varying rates of strain. Whilst simple elastic perfectly plastic material models are adequate for many applications, particularly where data is unavailable, they are unable to provide a wide ranging predictive capability. For modern materials, rate effects, thermal softening and path dependent behaviour are controlling factors in the deformation response to a shock wave. An accurate prediction of the post shock temperature is crucially important for modern material models, since the flow stress can be a sensitive function of temperature. Temperature also plays a crucial role in initiating and controlling localisation processes in materials. The accurate determination of temperature in turn requires an accurate pseudo-viscosity.

This paper describes work, performed under the auspices of the Anglo-French Defence Research Agreement, at DERA Fort Halstead and CEG, Gramat, to investigate the use of various pseudo-viscosity schemes for the treatment of shock processes. Whilst most studies have concentrated upon 'standard' test problems, this work directly addressed problems of interest to the research programmes.

Three schemes were considered: the classical scheme due to Von Nuemann, the modified scheme due to Wilkins and the more recent scheme due to Christensen.

The schemes were assessed against three simple classes of problem:

* 1 D plate impact of two copper plates
* the penetration of a copper sphere into a copper plate
* the collapse of an aluminium shaped charge liner

The results show that significant errors can arise in the prediction of the temperature with these schemes. This can result in quite marked differences in flow stress, particularly with modern material algorithms. In many cases the temperature can incorrectly place the condition of a material over its phase boundary.

The results of the study and the ranking of the various schemes, in terms of their ability to properly localise shock waves, are presented and discussed. The need for improved post shock temperature measurements is recognised and reviewed.

Finally the need for a tensor pseudo-viscosity to handle shear deformation is reviewed and ideas being developed are discussed. The ability to properly represent shear processes and their associated temperature dependency is a crucial requirement for a pseudo-viscosity scheme.

ADVANCES IN EXPERIMENTAL TECHNIQUES

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Over the past 100 years a range of techniques and sensors has been developed to follow the state of a material which has been dynamically loaded. It would be impossible to enumerate all of them here but we will aim to give an overview of the most commonly used sensors grouped according to the parameter that they measure. The aim of an impact experiment is usually to characterise the variables that describe the state of the impactor or target, in other words to define the pressure, volume and temperature as a function of time. Invariably these parameters are not measured directly. Instead related quantities such as stress, strain or particle velocity are. The range of embedded transducers and the more modern interferometric techniques is reviewed. New experimental arrangements for acquiring data that may be used to construct constitutive relations are reviewed.

MATRIX ISOLATION OF THE LASER INDUCED HIGH PRESSURE DECOMPOSITION OF RDX

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The pressure dependence of the laser induced decomposition of RDX (hexahydro-1, 3, 5trinitro-1, 3, 5-triazine) and RDX-d6 has been studied using a high pressure (up to 5.2 GPa) matrix isolation techniques in order to better understand the chemistry occurring under deflagration/detonation conditions. RDX samples were loaded in Merrill-Bassett anvil cells and cooled to a minimum of 23 K at the desired starting pressure. Each sample was exposed to a single 8 ns pulse of 532 nm light from a Nd-YAG laser. Thermal transport from the decomposing RDX into the anvils arrested the decomposition, trapping intermediates and products formed under high pressure-high heating rate conditions. The quenching rates and heat flow within the samples were estimated using a two dimensional finite element model. The technique was utilized to study single crystals, pressured powders and solutions to determine the effect of mechanical stress on the sensitivity towards laser initiation. The threshold energy for reaction initiation and product distribution is given as a function of pressure.

INITIATION OF PBX 9501 MEASURED WITH IN MATERIAL GAUGES

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Time resolved measurements of the initiation of PBX 9501 (density of 1.826 g/cm^3, about 98% TMD) have been made using in material electromagnetic particle velocity gauges. Sustained shocks were created by impacting the target with a Vistal faced projectile launched in a gas gun. Particle velocity histories were obtained at 11 depths ranging from the impact surface to 6 mm into the explosive.

The position of the shock/detonation front was also followed using a shock tracker. The waveforms clearly show the majority of the buildup is behind rather than at the shock front. In correlation with this, there is little acceleration of the shock front until detonation is achieved. These experiments provide a tight constraint on rate model calibration in reactive wave codes.

HYDRODYNAMIC INSTABILITIES IN SOLID IN MEDIA UNDER SHOCK LOADING

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Instabilities dividing heterogeneous media, which manifest themselves in high-velocity flows in liquid or gasses are well know. Among those are: Kelvin-Helmgoltz instability (slip instability), Rayleigh-Taylor instability (gravitational instability), Richtmeyer-Meshkov instability (boundary instability under shock wave effect). These instabilities have been studied faintly for solid media (or media featuring strength), although these cases are of special practical interest, namely, from the viewpoint of limitations associated with energy cumulation in pulsed inertial fusion systems.

The reports dwells on experiments aiming at study of the named instabilities at boundaries or free metals surfaces under shock wave loading up to 100 GPa amplitude or under high-velocity launching using HE-drivers of plane plates or converging shells.

Being discussed as well are methods and devices for experimental activities, diagnostic means and experimental results.

we have stated discontinuous nature of metal boundary behaviour at threshold amplitude shock wave failing onto it in normal conditions.

The reports analyses interconnection of instabilities development and metal turbulent mixing under shock wave impact with their strength and phase transitions, melting above all, caused by the same shock and subsequent rarefaction waves.

Several experimental results are being compared with their numerical simulations using different models of material behaviour under dynamic loading. The best co-ordination was fixed for viscouselastoplastic model, the dynamic yield strength and material viscosity of which depend on deformation intensity.

IMPROVED CYLINDER TEST AGREEMENT USING THE JAGUAR OPTIMIZED JCZ3 PROCEDURES

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The newly developed JAGUAR computer program utilizes advanced variable metric non-linear optimization routines to establish chemical reaction equilibrium by the minimization of the Heimholtz free energy of the system. Recently, the JAGUAR procedures for detonation properties of explosives have been extended for the calculation of detonation energies at adiabatic expansion conditions. The use of an extended JCZ3 equation of state with formally optimized EXP-6 potential parameters leads to improved agreement to detonation energies over TIGER JCZ3, BKWR and BKWC methods tested for relative volumes to 7.0. For the principal isentrope with C-J parameters and freeze conditions established at elevated pressures with the JCZ3 equation of state, best results

are obtained if an alternate volumetric relationship is utilized at the highest expansions. Efficient computer routines have also been developed which provide JAGUAR with the ability to automatically generate JWLB thermodynamic equation of state parameters. JWLB parameters were developed for TATB, LX-17, PETN, TNT, Octol, LX14 and PAX2A using the optimized JCZ3 parameters. The resulting JWLB equations of state were verified to closely reproduce experimental cylinder test results using DYNA2D finite element modelling, as well as providing agreement to the optimized JCZ3 predicted overdriven detonation behaviour.

TIME-RESOLVED OPTICAL SPECTROSCOPY OF TNAZ DECOMPOSITION AT STATIC HIGH PRESSURES DURING PULSE LASER HEATING

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An understanding of the chemical decomposition of energetic materials at high pressures and temperatures is essential in modelling shock wave processes in condensed media. Experimental measurements of fast chemistry at extreme pressures and temperatures, are crucial to attain this understanding. Chemical changes induced by rapid heating from a 8 ms pulsed laser operating at 514 nm was investigated to probe the decomposition processes associated with 1,3,3 tirnitroazetidine (TNAZ). The global decomposition rate and intermediate species produced are determined with from time-resolved absorption, emission, and Raman spectroscopy. The spectroscopic measurements were carried out at a maximum temporal resolution of 110 nanoseconds in the 400-700 nm wavelength region, during and up to 20 microseconds after the laser pulse. Above a threshold pressure and laser fluence, the reaction initiates and the TNAZ sample is consumed. The initial pressure and laser fluence correlates with the global reaction rates of TNAZ under extreme conditions. FTIR measurements from the reaction residue, were obtained and used to identify late time products of the reaction. TNAZ decomposition as a function of initial pressure and laser fluence is determined up to 5.0 GPa and up to 30 J/cm^2, respectively. The role of pressure and laser fluence on the initiation, the global reaction rate, the inferred reaction mechanisms, and implications on current models will be addressed.

MEASUREMENT OF RT AMPLITUDES AND WAVELENGTHS OF LASER DRIVEN PLATES*

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A laser driven plate, that is a dense solid plate driven by a laser heated, lower density plasma, is inherently Rayleigh-Taylor (R-T) unstable. In previous papers we have indicated that observed surface perturbations, on the plate, are probably R-T instabilities, initiated by the mode structure of the driving laser beam. A new experimental technique, using a semi transparent impact target viewed with a Polarized Epi-liluminated Confocal Streak Microscope, has allowed us to measure the amplitude and growth of the instability. The solid plate is deposited onto a quartz back plate, through which the drive laser is focused. The impact target having a semi transparent (semi reflective) coating, is separated from the plate by a fixed spacer. The reflective solid plate together with the target and spacer form an etalon, which when viewed at normal incidence, under laser illumination, produce interference fringes. When the initial accelerating shock breaks through the surface of the plate, its specular reflectivity is destroyed and the interference fringes disappear. Some time later the plate impacts the target changing its reflectivity. The streak image thus provides the temporal roughness of both the jump-off and impact of the plate. Knowing the velocity history of the plate

from separate VISAR measurements we can compute the amplitude of the instabilities at impact. The record also provides the time of flight, corroborating the VISAR measurements. By using spacers of different thickness, the growth of the instabilities can be observed.

Instabilities have been examined in both Aluminium and Titanium plates and the data will be discussed.

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NUMERICAL MODEL FOR SIMULATIONS OF DYNAMIC BEHAVIOUR OF COMPOSITE SHELLS UNDER EXPLOSIVE LOADING

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This paper presents the model and the numerical simulations of dynamic behaviour of shells manufactured from fiber composite material. This material was produced by helicalcircular coiling of ribbons from glass threads impregnated with epoxy binder. Testing of the numerical model was carried out using the experimental data on explosive loading of open cylindrical shells manufactured from fiber glass. We considered different variants of the material with different structure (the number of helical and circular layers, coil angles) and different levels of loading for these materials.

Approaches and models, available presently, provide opportunity to describe with sufficient extent of accuracy the behaviour of composite shells under small levels of strains at the stage of linear behaviour of material. As experimental data show the behaviour of such materials acquires non-linear character when the level of two-axial strains grows. The proposed model allows to obtain a satisfactory description of response of constructions (manufactured from composite materials) as in the region of small strains as in the region of large strains up to destruction level. The model takes also into account the condition of multiple loading of construction.

AN EVALUATION OF THE CERES PULSE POWER MACHINE FOR FLASH X-RAY CRYSTALLOGRAPHY

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CERES is a design for an electrical pulse power machine delivering a voltage of the order of 100 kV in a pulse about 10 ns long to an X-ray diode. It is hoped that CERES might be used for crystallography on experiments with shock waves. Initial experiments on the device characteristics are described and the quality of diffraction data is estimated to evaluate the design as a possible diagnostic.

PROGRESS IN SMOOTH PARTICLE HYDRODYNAMICS

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Smooth Particle Hydrodynamics (SPH) is a meshless, Lagrangian numerical method for hydrodynamics calculations where calculational elements are fuzzy_particles which move according to the hydrodynamic equations of motion. Each particle carries local values of density, temperature, pressure and other hydrodynamic parameters. A major advantage of SPH is that it is meshless, thus large deformation calculations can be easily done with no connectivity complications. Interface positions are known and there are no problems with advecting quantities through a mesh that typical Eulerian codes have. These underlying SPH features make fracture physics easy and natural and in fact, much of the applications work revolves around simulating fracture. Debris particles from impacts can be easily transported across large voids with SPH.

While SPH has considerable promise, there are some problems inherent in the technique that have so far limited its usefulness. The most serious problem is the well known instability in tension leading to particle clumping and numerical fracture. Another problem is that the SPH interpolation is only correct when particles are uniformly spaced a half particle apart leading to incorrect strain rates, accelerations and other quantities for general particle distributions. SPH calculations are also sensitive to particle locations. The standard artificial viscosity treatment in SPH leads to spurious viscosity in shear flows.

This paper will demonstrate solutions for these problems that we and others have been developing. The most promising is to replace the SPH interpolant with the moving least squares (MLS) interpolant invented by Lancaster and Salkauskas in 1981. SPH and MLS are closely related with MLS being essentially SPH with corrected particle volumes. When formulated correctly, MLS is conservative, stable in both compression and tension, does not have the SPH boundary problems and is not sensitive to particle placement. The other approach to solving SPH problems, pioneered by Randies and Libersky, is to use a different SPH equation and to renormalise the kernel gradient sums. An elegant theoretical framework for MLS is presented in a companion paper by G Dilts.

Finally we present recent results using the SPH statistical fracture model (SPHSFM). It has been applied to a series of ball on plate impacts performed by Grady and Kipp. A description of the model and comparison with the experiments will be given.

NUMERICAL SIMULATION OF FAILURE IN BRITTLE MATERIALS USING SMOOTH PARTICLE HYDRODYNAMICS

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At the Ernst-Mach-Institut (EM]) ductile and brittle materials are studied both by experimental and numerical means. The interest is focused on their properties under shock loading and on damage effects. Experiments by flyer plate impact, Hopkison bar, penetration and perforation on light gas guns provide basic input data for numerical investigation and allow to verify and adjust new attempts of constitutive modelling.

Hydrocodes are the basis of our numerical modelling. Besides use of commercial codes with standard Lagrangian and Eulerian spatial discretisation, an own meshless SPH code is currently

been developed. Applications range from low to hypervelocity impacts under consideration of ductile, porous and brittle materials.

Different material models based on micromechanic and continuum damage approaches as well as microstatistical modelling of inhomogenities are employed. Their performances of reproducing damage fracture patterns, crack front velocities and continued fragment loading in SiC and alumina ceramics are compared to experimental tests. Plates impacted by projectiles at one edge during observation by high speed cameras, flyer plate tests and deep penetration in confined targets allow consideration of different fracture conditions.

For brittle materials, the mechanical modelling and numerical discretisation of cracks turned out as one key problem for correct explicit simulation of damage, fracture and fragmentation. Nevertheless this represents the most promising feature of meshiess methods with their ability to reproduce very large strains, void formation, fragment rolling and ride up.

A NEW NUMERICAL SCHEME FOR SPH METHODS

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Some kind of problems appearing in terminal ballistic cannot be efficiently simulated with lagrangian and eulerian hydrocodes: for instance debris cloud produced by a hypervelocity impact or more generally perforation of a thin target by a kinetic projectile.

This paper describes the PhD work, realised in the CEG in association with Professor Vila from University of Toulouse. The subject is the study of the new particle method Smooth Particle Hydrodynamics (SPH).

Developed by Lucy, Monaghan and Benz for astrophysical problems later in the 70's, SPH has been applied to resolve Euler equations to study shock tubes or hydro dynamics applications. The SPH method uses no underlying grid. It is a pure lagrangian particle method. Due to the absence of mesh, SPH can handle large deformations. Each SPH particle represents a mathematical interpolation point at which all the fluid characteristics are known. The complete solution of the problem is obtained at all points in space by the application of an interpolation function. This function, the so called "cut-off" function, is required to be continuous and differentiable. One of the problem of SPH was the difficulty to simulate the rarefaction zones. This was due to the use of a constant variable smoothing of the cut-off function. One main improvement of the method, in the middle of the 80's, was the introduction of variable smoothing length which leads to the resolution of these problems.

We took as a basis one SPH code resolving Euler equations named Smart Fluids and developed by X-RS society. The first step was to incorporate material strength and the complete stress and strain tensor to study detonics and shock processes in condensed matter.

Our numerical simulations showed that computations could diverge and sometimes lead to non physical results. These observations have been proved by our mathematical analysis. As a matter of fact, the formulation, with variable smoothing length, written by Monaghan and al and used by the SPH community is not consistent. We introduced new concepts for use of variable smoothing length. They lead to the development of a consistent writing of the interpolation theory derived of the general ""scatter"" interpretation, and to conservative schemes. We proved the theoretical and

numerical convergence of our new scheme and we tested it on impact problems of two copper plates.

Hence, we applied these new developments and this new formulation to fracture and damage phenomena.

SMOOTHED PARTICLE HYDRODYNAMICS FOR SPACE DEBRIS IMPACT SIMULATIONS AN APPROACH WITH THE PAM-SHOCK TRANSIENTDYNAMICS CODE

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Space debris (hypervelocity) impact is a phenomenon of increasingly great importance for future spacecraft and satellite deployment missions. In this paper the process of virtual design of spacecraft shields is demonstrated using numerical simulations with the PAM-SHOCK family of codes which includes both Finite Element and Smoothed Particle Hydrodynamics (SPH) capabilities. First the basics behind the SPH approach as compared to the lagrangian one are described. Then, three basic scenarios are presented involving the impact of Aluminium projectiles on Aluminium targets, namely.. a spherical projectile impacting a Whipple shield at 6.6 km/s (normal impact) and cylindrical projectiles created from shaped charges and impacting a Whipple and a double bumper shield at 11.1 Km/s (both normal impact and 45 degrees inclined configurations). The latter two scenarios do currently represent the limits of experimental testing as far as propelling sizeable objects of a given structural integrity to such high speeds is concerned. The numerical simulations for normal impact were performed in both an axisymmetric space using the PAM-SHOCK2D code, which is a Lagrangian code with rezoning/remeshing capabilities and features dedicated to hypervelocity impact (eg SESAME EOS databank for a range of metallic, non-metallic and composite materials) and in a full 3D space using PAMSHOCK with the SPH option. The 45 degrees inclined impact simulations were performed in 3D with the SPH option. The results obtained focused on the correct representation of the bumper penetration process, the debris cloud composition, kinematics and evolution and the subsequent damage inflicted to the backwall (spacecraft). A comparison is given of the numerical results for SPH against the experimental results and the Lagrangian solution results where applicable. Some interesting numerical experiences are shared and finally the benefits of the SPH approach for arbitrary 3D impact are exposed. The work is currently continuing with non-metallic composite targets (Nextel and Kevlar materials). The emerging results will be exposed in due course.

SPH TECHNIQUES AND THEIR APPLICATION TO IMPACTS ON BRITTLE MATERIALS

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SPH (Smooth Particle Hydrodynamics) is being increasingly used for modelling many large deformation transient dynamic problems. For some applications, notably hypervelocity impacts on thin plates, SPH techniques appear preferable to conventional grid based Lagrangian and Eulerian techniques. For many other applications SPH shows promise which may be realised when improvements are made to the method. Unlike grid-based Lagrange, SPH does not suffer from problems of grid tangling and the need to use erosion and rezoning algorithms. Practical advantages

of SPH over Euler techniques are computational cost and flexibility in incorporating constitutive material models.

The implementation and application of an SPH capability in the hydrocode AUTODYN-2D has been presented previously [1], [21, [31. The implementation incorporated published features which were either common to, or sometimes unique to, other SPH implementations ([41, [5], 161, [7] and [81). We found that the performance of some SPH technology, at that time, was not as good as was sometimes suggested in the literature. We will outline these findings and present solutions that were developed to overcome some of these deficiencies. Successful and unsatisfactory validation simulation results will be presented.

SPH, as a relatively new technique suffers from some significant problems that are being increasingly recognised. In an effort to overcome these problems new work has been conducted [91, [1 0] which purports to solve many of the problems associated with the method. The experience of the authors with these new techniques will be presented. In particular the presentation will focus on our experiences of implementing and using methods which are aimed at solving the consistency and stability problems of SPH.

In order to illustrate the practical application and benefits of SPH, calculations will be presented and compared with well characterised experimental cases. The emphasis will be on applications related to impact on brittle materials such as glass and concrete; a sample output from an SPH simulation of ceramic impact is shown below. Conclusions drawn from experience with damage and fracture models such as the Johnson-Hoimquist brittle model (11), will also be made.

NEW DIRECTIONS IN SPH

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It has been observed that the standard formulation of SPH can show instability in tension and inaccuracy in gradient estimates when the particle spacing becomes irregular. These problems have now been resolved. The instability is effectively removed with a particular form of artificial dissipation called conservative smoothing. The inaccuracy has been removed with kernel renormalization. These remedies will be discussed and assessed.

The renormalization procedure leads one to a new formulation of SPH that is quite different, philosophically and numerically, from the original implementation. First of all, the renormalization of the accelerations requires one to use the stress difference form of the momentum equation, which also helps substantially in correcting the instability problem (standard SPH uses the stress sum form). Secondly, the increase in accuracy afforded by the renormalization requires one to treat the boundary surface particles explicitly. Customary impact problems simply will not run if boundaries are ignored, as has been the case in standard SPH.

We conclude, therefore, and will discuss in detail, that important recent improvements in SPH have focused attention on the boundaries where both free-surface and contact conditions must be treated with great care. Current progress in our implementation of boundary conditions in SPH will be discussed. Of particular interest is how our damage and fracture models interact to form new stress-free boundaries. Several examples of simulated fracture and fragmentation using the new SPH paradigm will be presented.

THE-MOVING-LEAST- SQUARES-PARTICLE HYDRODYNAMICS METHOD

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An enhancement of the smooth-particle hydrodynamics (SPH) method has been developed using moving-least-squares (MLS) interpolants which simultaneously eliminates or significantly mitigates several well-known undesirable behaviours of the SPH method, including spurious boundary effects, inaccurate strain and rotation rates, and the infamous tension instability. The classical SPH method is derived in a novel manner by means of a Galerikin approximation applied to a special form of the Lagrangian equations of motion for continua. This derivation is then modified in a trivial manner to introduce the MLS interpolants, resulting in the MLSPH method. Particle masses and volumes must be carefully redefined. A new method for detecting boundaries very naturally falls out of the treatment. The improvements in several severe test problems are quite dramatic. Performance issues are addressed.

UNRESOLVED PROBLEMS AND NEW DIRECTIONS IN THE SHOCK WAVE PHYSICS OF METALS

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CONTINUUM AND SUBSCALE MODELLING OF HETEROGENEOUS MEDIA IN THE DYNAMIC ENVIRONMENT

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Systems and structures designed to function in the severe dynamic environment are increasingly relying on the use of high-performance composite materials. Such materials can include both benign materials selected for unique strength or response characteristics under dynamic loading or active materials in which the dynamic event stimulates molecular change or energy release features critical to the system performance. A metal-ceramic composite would be representative of the former while the later might be characterized by a plastic-bonded explosive The superior performance of composite materials involves unique material features on multiple scales ranging from the molecular through the micro- meso- and macro-scale of the media. These materials can be heterogeneous, nonlinear, random or layered and anisotropic. Material engineering on the subscale may involve unique strength enhancement techniques or may impart active physical response features such as phase transformation or chemical reaction. Such systems will be subjected to, and required to perform under, intense impulsive loads. The assessment and evaluation of the response of these systems to complex loading conditions will ultimately require advanced computational methods relying on accurate physics-based material models. Analysis provided by such computation techniques and modelling methods must forecast, not only propagation of gross momentum and energy imparted by the impulsive load, but also track the evolution of energy through internal subscale degrees of freedom when these coordinates actively participate in the material and system performance.

The present effort is directed toward the development of a physics-based model for heterogeneous composite materials for the expressed purpose of addressing the problems suggested above. Of particular interest are large-amplitude, wave-dispersion characteristics and the excitation of internal degrees of freedom brought about by the multiscale heterogeneous nature of composite media. The modelling effort focuses on nonlinear, heterogeneous matter and explicitly address the evolution of incoherent (scattered) energy responsible for subscale physical phenomena in the dynamic event as well as the continuum wave propagation properties. Specifically, a normal mode representation of matter is used to describe the nonequilibrium and incoherent acoustic energy stimulated by a finite amplitude shock wave. Laws of stimulation and relaxation toward statistical mechanical equilibrium are developed which lead to continuum anelastic models for the dynamic response. In the present paper a model is developed in which two dominant modes important to the substructure physics are coupled, leading to additional character in the processes of relaxation toward equilibrium. The model is used to examine the nature of steady structured shock waves in solids.

SPALLATION MODELLING IN TANTALUM

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A gas gun plate impact spallation experiment has been performed on commercial purity rolled tantalum. The shock pressure achieved was about 7 Gpa and was sufficient to induce incipient spallation. The particle velocity was measured at the free surface of the spalled plate, and the spalled sample was recovered and examined metallographically using image analysis. The quantitative image analysis results have been utilized in a spallation damage model. The model is micromechanically based and involves novel void growth and coalescence processes. Here we report the results of hydrocode calculations of the gas gun plate impact using this model. The 1 D characteristics code CHARADE has been used to simulate the VISAR free surface particle velocity record. Implications for ductile damage modelling will be discussed.

THE RELATION BETWEEN THE DEFORMATION MODES OF LONG-ROD PROJECTILES AND THEIR PENETRATION CAPABILITY

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Penetration mechanics of long-rod projectiles has been the subject of intensive research over the last 30 years. On the practical side, rods of increasing lengths and densities have been developed, reaching penetration depths of 0.5 m in armor steels. On the theoretical side, both analytical models and numerical simulations were developed in order to better understand the processes involved in these interactions. One of the main conclusions of these theoretical efforts was that the strength and failure mode of the rod have secondary importance on their penetration capability, adopting a quasi-hydrodynamic description of the process. However, recent experiments, performed in the last decade, have shown that the penetration process of dense long-rods (made of tungsten alloys and depleted uranium) is far from hydrodynamic, and that the failure mode of the rod material plays an important role in the process.

The purpose of the present paper is to summarize our recent work on this subject, using two-dimensional numerical simulations with the Eulerian processor of the PISCES-2DELK code. We

investigated several issues influencing the penetration process which include, the yield strength of the penetrator, its maximum strain to failure, the temperature softening at the penetration tip due to large deformations, and the influence of the hose shape on its penetration. Our results show that with increasing yield strength, an optimum is reached in the penetration depth vs. rod strength curve. The optimal strength depends on impact velocity increasing from 0.8 GPa at 1.4 km/s to 2.5 Gap at 2.2 km/s. When temperature softening is added to the constitutive relation of the rod material, these optima are replaced by an asymptotic behaviour. Thus, we conclude that with real long-rods (which soften at their tips), it is unnecessary to unnecessary to increase the strength of the rod beyond a certain value, as far as depth of penetration is concerned.

The role of maximum strain to failure ($\in_F$) is very interesting since, as it turns out, there is a large drop in penetration depth for $\in_F$ in the range of 0.2-0.5. The magnitude of this drop decreases as impact velocities are increased. These findings can explain the differences found between the penetration depths of tungsten alloy and depleted uranium long-rods. These differences were attributed by L Magness and his colleagues (at ARL) to the adiabatic shear failure at the tip of the uranium rod, which leads to a self-sharpening process of this tip. The differences between penetration capabilities of these two materials diminish with increasing impact velocities. Thus, our simulations strengthen these interpretations and also lead to an explanation for the geometrical-nonscaling issue which was recently found for these penetrators. in order to further explore these issues, we performed a set of simulations with rigid penetrators having different nose shapes. These resulted in a large range of different penetration depths giving more support to the selfsharpening hypothesis.

MESOMECHANICAL APPROACH FOR DESCRIPTION OF SHOCK WAVE LOADING IN SOLIDS

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The approach connecting processes of the material deformation on micro- and mesoscale levels is developed. The construction model allows to retrace process of shear bands formation under shock-wave loading. The possibility of appearance of the internal moments caused anisotropy of properties on micro- and mesolevel takes into account in this model. So, limitation of the number of activity slip planes in the metal grains calls forth its rotation and shear bands formation already in the shock wave front. Accommodative deformation of the material mesovolumes is caused by evolution of the dislocation continuum.

The results of computer simulation of plastic deformation of the mesovolumes are represented.

PLASTIC STRESS WAVE IN METALLIC POWDERS DUE TO LONGITUDINAL IMPACT

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Dynamic powder compaction is considered as one of the most effective methods to break surface oxides of metallic powders such as aluminium, magnesium etc. Breaking oxides is indispensable to achieve good sintering.

In this paper, the wave propagation including smooth stress waves and shock waves in metallic powders is studied to make clear the dynamic powder compaction process.

Rapidly solidified Al/Li powder (mean particle size-. 64.2 μ m) is uni-axially compacted by static and dynamic methods and sintered experimentally. Transient electromagnetic force is used for the dynamic powder compaction. Better mechanical properties are obtained by the dynamic compaction and sintering.

A computer program is developed to simulate the dynamic powder compaction process. Characteristic curves are derived from equation of motion, constitutive equation and compatibility equation, and the numerical integration is carried out along the characteristic curves by Hartree method. First of all, the validity of the program is confirmed by the comparison between analytical and experimental results in terms of strain distribution along the Lagrangian coordinate X.

The plastic wave propagation in the powder is studied using the computer program. The influence of friction between powder and container, loading conditions, reflection at the impact tool, length and initial density of the specimen, etc on the plastic wave propagation is estimated by using the program. The temperature rise due to the plastic work and the friction is also estimated.

As a result, followings are obtained. The wave reflection between tool surfaces should be effective to break the surface oxide of the powder. Plastic wave changes its shape by the development of secondary stress wave during unloading process. Friction and temperature rise reduce the possibility of forming plastic shock waves significantly. The temperature does not rise so much during the dynamic powder compaction process.

IMPACT OF ALUMINA - A COMPREHENSIVE STUDY

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Shock-wave techniques combined with time-resolved instrumentation methods play a crucial role in understanding the transient deformation features of materials. This is particularly true for ceramics which display unique characteristics associated with the dynamic deformation process. What makes the ceramics particularly interesting is that they are brittle, strong in compression, but weak in tension.

There is a need for accurate ceramic material models to facilitate computational and engineering analyses involving ceramic materials under dynamic loading. Well-controlled impact techniques and high-resolution diagnostics are generally used to determine the baseline material property data, often under uniaxial strain conditions. This is the first step necessary to determine the equation-of-state and constitutive material properties such as the yield strength or fracture strength of materials under transient loading. Such a data base forms the foundation for material models that have been developed for engineering analysis in computer codes.

Validation and the continued development of ceramic material models appropriate under multi-axial loading conditions will, however, requires the existence of a comprehensive material property data base. It is the purpose of this paper to report measurements on alumina under a broad range of dynamic loading conditions. Gun experiments, combined with velocity interferometric techniques, have been used to experimentally determine the loading behaviour of a Coors-AD995 alumina. Alumina is highlighted in this paper because it is material that has been studied extensively both

to probe the material for failure waves will also be discussed. These experiments are expected to form a data base to stimulate the development of a multi-dimensional constitutive model needed to simulate dynamic impact events in high-performance computer codes.

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MODEL OF CONSTRUCTIONAL CERAMICS MECHANICAL BEHAVIOUR UNDER SHOCK LOADING

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The modern constructional ceramic materials have a high strength, sometimes greater by several times then metal allows.

The constructional ceramics experiences an inelastic deformation under loading as a high strength alloys.

An inelastic deformation about 5-10% develops before fracture of silicon and boron carbide ceramics and alumina. That is why the brittle materials model is not correct for the constructional ceramics. Strengthening and dissipation of the mechanical energy effects may be connected with different physical micromechanisms.

The model of one phase polycrystailine ceramics behaviour under shock loading is presented in this report. The development of the macroscopic inelastic deformation is determined by the growth of pre-existed microcracks.

The model is based on the continuum mechanics and solids are represented by the elastic-visco-plastic damage continuum.

Shear stresses are calculated from the relaxation equation where the effective inelastic deformation is defined by the kinetic equation concerned with cracks growth. It is assumed that the microcracks specific number is a constant but the average cracks radius depends on the loading history. Every ceramic specimen has many penny shaped microcracks which were originated during specimen manufacture.

The transcrystalline fracture takes place in many polycrystalline ceramics. In this case the tip of the microcrack moves on the grain boundaries. The friction gives additional resistance to the growth of shear cracks under shock loading and this factor is taken into account in the kinetic equation. The microcracks grows and opens under tension that leads to advent of the bulk inelastic deformation and rise of damage parameter.

The damage parameter is defined as specific volume of crack's spaces. The criterion of the fracture is the equality of the damage parameter to its critical value.

The model was used for simulations of plane shock wave propagations in boron and silicon carbide ceramics. The calculation results have a good agreement with experimental data. The model may be applied for solving two-dimensional tasks with sufficient relaxation phenomena.

A CONSTITUTIVE MODEL FOR REPRESENTATION OF PROGRESSIVE DAMAGE AND FRACTURING IN BRITTLE MATERIAL SUBJECTED TO HIGH STRAIN RATES

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Ceramic materials are increasingly being used for components subjected to high strain rates where high-energy absorption is a desirable characteristic. Characterisation of the performance of such materials via experimental testing is difficult and expensive so that representation using a computational model that captures the fundamental mechanisms. Of their response offers large benefits.

In addition to modelling the evolution of damage in the ceramic material, projectile impact simulations provide additional challenges because of the need to simulate finite deformation plasticity associated with the projectile deformation contact interface mechanics between the penetrator and the ceramic and between ceramic particles if fragmentation is represented.

This paper outlines a new constitutive model based on finite/discrete element analysis that characterises the behaviour of brittle materials e.g. concrete and ceramics, when subjected to high strain rates in both tensile and compressive regimes. The model represents the degradation of the material's strength via a damage-based micro-crack growth law exploiting fracture energy concepts and including the effect of the rate of nucleation and micro-crack coalescence. The dependence of the model on fracture kinetics is essential for high strain rate regimes where brittle materials can sustain compressive stresses much higher than the quasi-static compressive strength. The local constitutive model is coupled to a macroscopic fracture propagation algorithm that enables fracture of the initial intact material into small fragments, whose interaction is governed by a general interface law.

Unlike the more generally applied continuum approaches, the current model is able to represent the performance of the ceramic material in both its initial intact state and after fragmentation and can include complex phenomena such as:

dilatancy due to crack opening damage induced anisotropy
residual strength due to frictional interaction of fractured particles

The paper will briefly describe the model and then illustrate its effectiveness in simulating both small and large-scale experimental tests including various animated projectile impact examples.

NUMERICAL MODELLING OF TWO PHASE REACTIVE FLOW AND ALUMINISED EXPLOSIVES

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We consider the problems of numerical modelling of the detonation and subsequent explosion of an Aluminised explosive. The presence of reactive Aluminium particles complicates the modelling in two main ways. The first is hydrodynamic since we have to allow for the interaction of solid Aluminium particles with the flow of the surrounding explosive and its products. We thus need to account for interphase heat and momentum transfer (e.g. conduction and drag effects). The second additional complication is due to the relatively slow burn rate of the Aluminium particles when compared with the energy release of a high explosive.

We introduce the basic equations and method of solution we have adopted in an Eulerian Multi-material hydrocode.

We also present results of calculations of supporting experimental studies and relevant results from the literature on detonation and combustion of clouds of Aluminium particles in Air.

PRESSURE EFFECT ON COMBUSTION WAVE IN SOLID POROUS MEDIA

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The present work is devoted to investigation of combustion wave propagation in porous media. The main feature of the process is correlation between temperature and pressure elevation due to viscous gas flow in the medium. The structure of the combustion wave and its velocity as well as temperature and pressure values behind the wave front are obtained.

The solid porous media fulfilled with combustible gas mixture is considered. We restrict ourselves to the case of the combustion wave which propagation is controlled not by heat and mass duffusivities but rather by the adiabatic compression. The latter is supported by the energy release provided by the exothermic oxidation reaction. Our main goal is to determine a velocity of combustion wave propagating in the porous medium under an assumption that creeping flow of viscous gas is realized. We use the physical model which was suggested by Goldshtein et al (1994) for a description of the combustion wave propagation driven by pressure diffusion. Governing relations include energy, concentration, state, continuity equations for the gas phase as well as Darcy's law for viscous gas flow. We believe that chemical kinetics of the oxidation reaction is obeying Arhenius law for the one step reaction of the first order.

The problem investigation is performed by application of synthesis of physically reasonable assumptions, analytical asymptotic geometric method (integral manifold method) and numerical calculations. In the dimensionless variables, which are conventional for the thermal explosion theory, the original system is reduced to a form of singularly perturbed system. The system is multiscale: temperature is the fast variable, concentration is slow and pressure is an intermediate one. A relation between combustion wave velocity and gas pressure behind the wave front has been obtained as a result of an analysis of the system trajectories behaviour in the phase space.

Introduction of additional assumption concerning existence of a narrow reaction zone permits us to apply the approach suggested by Goldshtein et al (1 994) for the further system examination. As a final result we obtain an implicit functional equation with respect to the gas temperature behind the wave front. The functional equation is solved numerically and values of the temperature and pressure (behind the wave front) as well as combustion wave velocity are obtained as functions of initial conditions and main physical/chemical parameters of the system.

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MULTIPLE REACTION RATE DETONATION MODELLING

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The ability to model non-ideal detonations includes the ability of the modelling to handle energetic materials which have multiple reactions involved in their release of the chemical energy during the detonation. The modelling of the energy release due to multiple reactions becomes critical to the characterization of the blast at distance from non-ideal explosives which may be used by terrorists. First, a portion of the energy is released within a region wherein the local sound speed is greater than the flow velocity which allows this energy to catch up with the initiating shock wave and maintain its steady support. Correctly modelling this energy release requires the modelling of multiple independent and/or dependent reactions which demands a change in the method of handling the mixed phase physics in the computer code. A second problem imposed by the multiple reaction rates of a non-ideal explosive is the problem of calculating the expansion of the pressure from such an explosive when a significant portion of the energy is not transferred into the air by the shock wave. This means that the usual isentropic expansion may not be used until all of the energy released by the slower reactions catches up with the shock wave in the air and the final entropy of the combination of the air and reaction products may be determined.

This presentation will discussed these problems and the approach taken toward their solution as well as the current status of the research.

MODELLING EXPLOSIVE SHOCK INITIATION IN MULTI- DIMENSIONAL LAGRANGIAN AND EULERIAN HYDROCODES

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At AWE, shock initiation modelling of solid heterogeneous explosives is performed using the Ignition and Growth reactive flow model developed at the Lawrence Livermore National Laboratory. This model has been incorporated into in-house multi-dimensional Lagrangian and Eulerian hydrocodes.

The phenomenon of desensitisation of an explosive by a weak preshock is currently of interest. Considerable experimental evidence has been accumulated which shows that initiation and run distance to detonation can be significantly modified by preshocking. The shape, amplitude, and duration of the preshock are all important contributors to the explosive response.

The Ignition and Growth model to predict explosive response to shock loading is derived from single shock data, and hence had not considered the effects of shock desensitisation. To take account of this phenomenon, a simple but physically realistic desensitisation model has been developed within the confines of the Ignition and Growth model. This simple model is described, and calculational results are compared with some of the available experimental data.

To study high explosive response to shock loading, an experimental vehicle has been developed at AWE. The vehicle consists of a donor explosive charge that is used to shock an acceptor charge through an inert barrier. The system is confined by stainless steel and perspex. PVDF gauges are used to provide quantitative in-situ pressure measurements in the shocked acceptor charge, giving reaction rate information on explosives of interest.

A series of cylindrical geometry shock initiation experiments have been performed using this vehicle to examine the shock sensitivity of the high explosive formulation EDC37, which contains 91 % by weight HMX, 8% KlO liquid, and 1 % Nitrocellulose. An Ignition and Growth reactive flow model for EDC37 has been developed from the available experimental data.

DETONATION AND TRANSITION PROCESSES IN LOW-DENSITY EXPLOSIVE SYSTEMS

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Both experimental and theoretical results on initiation and propagation of detonation and nonsteady reactive shock waves in two-phase gas-solid (or liquid) explosives of density amounting to 8 kg/m^3 are presented. Considered are both suspensions of powdered materials in air and layers of explosives materials spread over the tube floor. The explosive materials used in experiments were: RDX, HMX, TNT, and mixtures of Al with ammonium nitrate or ammonium perchclorate.

The process was monitored using a streak camera and pressure gauges. The minimum energies of direct detonation initiation and pressure profiles behind the reactive shock waves were measured. The results are compared with thermodynamic calculations of the parameters of CJ detonation in the mixtures.

The studies of detonation wave initiation in tubes have revealed the following peculiarities of the process: (a) parameters of the detonation waves are always lower than thermodynamically calculated ones, (b) TNT in suspensions turn out more detonable than RDX and HMX, (c) detonation waves exhibit essentially nonideal behaviour-. two-front detonations and detonation waves with local explosions behind the lead front are observed, (d) in mixed, layer suspension systems detonation is initiated in two stages in the form of a weak and strong detonation waves following each other at different velocities, (e) detonation in suspensions is very hard to initiate at initial room temperature, but preheating the mixture with a weak detonation or shock wave drastically shortens the distance to detonation.

Characteristic times of powder lofting and particle burning behind shock waves are determined experimentally. The times were incorporated in a 1 D code to simulate the initiation process. Two-dimensional calculations of the material lofting behind shock waves agree fairly well with experiment.

APPLICATION OF A VISCOPLASTIC PORE-COLLAPSE MODEL TO THE SHOCK INITIATION MODELLING OF EXPLOSIVES

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At the TNO Prins Maurits Laboratory a research programme is being carried out on the characterisation and development of less sensitive explosives. The influence of the properties of the RDX crystals, such as the particle-size and -shape, on the shock sensitivity of RDX-based PBX's is investigated, applying both shock pulses generated by an explosive charge in a gap test geometry and shock pulses generated by the impact of high-velocity flyers. Besides the experimental work on the formulation and testing of the explosives, computer simulations are being performed in order to reach a better understanding of the experimental data on shock initiation. On the one hand the modelling work aims at the description of the differences in initiation behaviour between shocks of different length and shape, corresponding with the applied experimental initiation techniques. On the

other hand the influence of the size and the size distribution of the explosive particles on the shock initiation behaviour is being studied.

The simulations are carried out with the hydrocode Autodyn. Initially the Lee-Tarver model, which is intrinsic to Autodyn, has been used for shock initiation modelling. In this semi-empiric initiation model the initiation process is split into two stages, an ignition stage where the explosive particles are ignited, and a growth stage, where the particles are burned. Although some aspects of shock initiation can be described very well with the Lee- Tarver model in Autodyn, the model has appeared to be inadequate in the explanation of the experimentally observed dependency of the initiation behaviour on the explosive particle size'. Especially the description of the ignition phase in the model is in sufficient.

In order to improve the description of the shock initiation process the model has been adjusted by making use of the so-called visco-plastic pore-collapse model for the ignition stage. In such a model the creation of hot spots due to visco-plastic flow during the collapse of cavities in the material and the subsequent ignition of the particles are described. From several pore-collapse models, reported in the literature, the model of Khasainov *et al*[2] has been selected for implementation in Autodyn. Because of the restraints, imposed by the hydrocode, it is not possible to incorporate the model directly into the hydrocode. Therefore an expression has been derived for the average reaction rate during the ignition stage, applying some expressions given by Khasainov *et al,* which then replaces the ignition term in the Lee-Tarver model, while retaining its growth terms.

With the revised shock initiation model a series of simulations has been performed where both the pulse height and the explosive particle size have been varied. The results are generally better than those obtained with the previous model and it has appeared possible to explain qualitatively some particle size effects, that have been observed experimentally. The first results with this provisional model have demonstrated its potential for explaining shock initiation phenomena.

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COMBUSTION WAVE PROPAGATION IN A MULTIPHASE MEDIA

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A novel approach to multiphase laminar combustion waves is presented. Specifically, the proposed method allows to obtain reasonable approximations of flame structure, to calculate numerically flame velocity and to estimate the maximum combustion temperature.

The main physical point is that the reaction (combustion) zone of the flame is analysed in detail, by comparison with the classical methods (E.g. Zeldovich et al. And Frank-Kamenetskii). This has a great importance for multiphase systems where interaction between the phases leads to considerable complication of the flame structure. The mathematical point is applications of the fast

("adiabatic") integral manifolds of the pertinent mathematical models and analysis of the self-ignition phenomena involved.

For illustrating the method, a system of combustible gas with addition of inert liquid droplets is considered. In particular the effect of liquid droplets on the wave profile is studied. It is shown that the temperature profile becomes more complicated. Specifically there is a possible temperature drop in the reaction zone.

MOLECULAR DYNAMICS SIMULATION

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Computer simulation offers a way of examining crystal structures under conditions of extreme pressure which may be difficult to obtain in a controlled way experimentally. The {\it ab initio} calculation of equations of state, using a parallel supercomputer to simulate extreme pressures and temperatures will be reviewed.

Application to a simple system, aluminium, will be described in order to present the method, then the treatment of more complex materials which exhibit phase transactions (silicon, carbon, strontium, silica) Will be discussed. The importance of the phase transition mechanism in determining whether thetransition will actually occur on the timescale of a shock wave will also be discussed: We demonstrate that the relevant equation of state may not be the equilibrium one, but that containing only those phases kinetically accessible.

A *PRIORI* CALCULATION OF COMPLEX LIQUIDS SHOCK POLAR BY QUANTUM CHEMISTRY AND MOLECULAR DYNAMICS SIMULATIONS

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We present in this paper a cheap method to determine shock polar of inert organic liquids. This method is based on quantum chemistry calculations associated with molecular dynamics simulations.

Equilibrium geometry of isolated molecule and associated normal vibration modes are calculated with a quantum chemistry code and compared with experimental data (X-ray diffraction, infrared and Raman spectra). The intramolecular potential function is a quadratic function of internal coordinates (interatomic distances, etc) and the corresponding force's constants are directly calculated from theoretical normal coordinates. Intermolecular energy is obtained with the supermolecule method in which two molecules are taken into account. It is deduced from many random intermolecular distances and relative orientations. The intermolecular energy is then fitted with an appropriate function which depends on all intermolecular interatomic distances. Finally, the two previous potential functions are included in a tridimensional molecular dynamics code.

To initiate a molecular dynamics simulation, we start from a regular structure at experimental liquid density and perform calculation until disordered phase is reached. Then, shocks of various intensity (defined by the average particle velocity u behind the shock) are applied to the system. The thermodynamic parameters are density p= 11V, temperature T and pressure P are deduced from positions, velocities and accelerations of the particles. The shock velocity D can be obtained from

time evolution of the average particle velocity profile. We check that *u, D,* p and P are consistent with Hugoniot relations. It is interesting to note that in our approach only the experimental initial density is necessary.

The previous method is applied to three systems: liquid nitrogen N2 at 75K, carbon tetrachloride $CC1_4$ (300K) and nitromethane CH_3NO_2 (300K), a liquid explosive. The P(V) and *D(u)* calculated curves are in good agreement (a few percent) with experimental data for nitrogen and nitromethane Result is not so good for CC14. Because both pressure and temperature are straightforward function of the time particle evolution, it is clear that shock's temperature can be extract of molecular dynamics calculations with the same precision that pressure. Our method is a very simple way to evaluate shock's temperature, which is well known to be difficult to measure in shock experiment.

So we have then shown that quantum chemistry associated with molecular dynamics simulations can be a very interesting way to determine quantitatively the thermodynamic state *(P, V,* 7) of a complex liquid under shock.

MOLECULAR DYNAMICS STUDY OF EFFECT OF TEMPERATURE AND STRUCTURE DEFECTS ON THE MAXIMUM STRENGTH OF CRYSTAL LATTICE

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The influence of structural defects and initial temperature on the maximum strength of the iron and copper crystal lattices has been studied by the method of molecular dynamics. The dependencies of the maximum strength of the iron crystallise on initial temperature and on the defect concentration such as vacancies and "helium-vacancy" complexes have been obtained for two-dimension and three-dimension crystallises. The temperature range of transition from brittle fracture to viscous one has been established for the two-dimension iron crystallise.

The time of structural relaxation of a metal lattice in a strong wave of compression has been determined by the molecular dynamics simulations. The curves of "cold" compression of the ideal iron crystallise and the iron crystallise with defects such as "helium-vacancy" complexes were calculated. It has been shown that at the defect concentration > 2.5% the "cold" compression curve differs appreciably from the "cold" compression curve of the ideal iron crystallise.

Structural instability of the crystal lattice was detected in condition of one-dimension compression of the three-dimension iron crystallise at value of a longitudinal stress about 17 GPa. In the specified stress-deformation conditions a transition of the lattice from cubic to hexagonal structure takes place.

SHOCKWAVE-INDUCED PLASTICITY VIA LARGE-SCALE NONEQUILIBRIUM MOLECULAR DYNAMICS

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In nonequilibrium molecular-dynamics (MD) simulations of shock waves in single crystals, carried out in 1979 at Los Alamos (1), we discovered that, above a threshold strength, strongly shocked crystals deform in a very simple way. Rather than experiencing massive deformation, a simple slippage occurs at the shock front, relieving the peak shear stress, and leaving behind a stacking fault. We

realised, of course, that real materials could yield at much lower thresholds, and speculated then that preexisting defects could nucleate plastic flow at lower shock strengths than those characteristics of pure single crystals. (Historical note: at about the same time as our earliest dynamical shockwave simulations, Mogilevsky, working independently in the soviet Union, carried out relaxation MD calculations under uniaxial strain, and observed spontaneous production of dislocations (2).

Further Los Alamos calculations, carried out nearly a decade later in five-times larger systems (up to 10,000 atoms), confirmed this observation and quantified the threshold strength, namely the yield strength of the perfect crystal (3). Subsequently, Zaretskii and c-workers (4). Using x-ray diffraction of shocked single crystals, confirmed our MD observations of stacking faults produced by shockwave passage.

With the advent of massively parallel computers, we have recently studied systems with over six-times larger cross-sectional area and for-times longer distance of run to the steady state (Approximately 270,000 atoms). We have seen that the increases cross-section allows the system to slip along both available forward lip systems, in different places along the now non-planar shock front, though only one stacking fault survives. This leads us to attempt simulations with even larger cross-sectional area, and with preexisting defects embedded in the sample, such as those we will report on here (36-times larger cross-sectional area: 10 million atoms). We report on shock waves in fcc copper, where the atoms interact via an EAM (embedded-atom-method) many-body potential, as well as pair-potential materials (5).

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MODELLING OF INITIATION, GROWTH AND DETONATION AT THE MOLECULAR LEVEL

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This paper will address the requirement for molecular level modelling of detonation processes. Various approaches to the problem will be described, and the difficulties of bridging length and timescales of interest with those which are accessible to fundamental studies will be discussed. Finally, the methods being developed at DERA will be described in some detail, and example calculations given.

In particular, the paper will concentrate on the use of molecular dynamics (MD) to study the fundamental interactions between shock waves and the chemistry of energetic systems. 2 and 3D simulations of "model" materials will be described and comparisons drawn with classical initiation models. These simulations make use of empirical inter-atomic potentials of Abel-Tersoff form. Additionally we will describe some preliminary studies of shock-induced reactions using an ab-initio quantum mechanical MD technique.

A REVIEW OF CONSTITUTIVE/DAMAGE MODELS FOR CERAMIC MATERIALS IN HYDROCODES

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This paper presents a comprehensive review of constitutive/damage models suitable for describing the high strain rate and shock response of ceramic materials in shock-wave propagation based finite element/difference numerical codes (hydrocodes). Since constitutive and damage models for ceramics are rarely available in hydrocodes, recently a few models have been implemented into different hydrocodes. Johnson and Holmquist (J-H) [1] considered a phenomenological approach in their model formulation. The strength variation with respect to pressure, strain rate, and damage was modelled using a set of empirical relationships. Steinberg [21 adopted his metal model equations for high pressure dynamic loading to describe the impact behaviour of ceramics. In this model, the compressive yield strength and shear modulus are varied with respect to pressure and temperature. Steinberg successfully reproduced the measured velocity histories from plate impact experiments for various ceramic materials. Rajendran and Kroupa [3] presented a ceramic model in which they assumed an elastic-viscoplastic behaviour for compressive loading and microcracking behaviour for tensile loading. In general, attributing the inelastic strains entirely to dislocation based plastic flow is not appropriate for brittle ceramics. Addessio and Johnson (A-J) [41 presented a microphysical model to describe the complex behaviour of ceramics. In their model, the inelastic strain is assumed to be due to microcracking of the ceramics. They modelled both crack opening under tensile pressure loading and crack sliding under compressive pressure. Espinosa et al [51 reported a multiple-plane crack model is which damage is assumed to evolve due to microcracks in nine independent orientations. Recently, Rajendran [61 reported a continuum mechanics based three dimensional constitutive model (R-G model) to describe the impact behaviour of ceramic materials. This model is based on microcrack nucleation and growth, as well as pore collapse mechanisms. Damage is defined in terms of an average crack density and is treated as an internal state variable. The various model developers used the plate impact experimental data of Kipp and Grady [71 to validate their respective model constants. This paper also presents a comparative study of Steinberg, J-H, A-J, and R-G models in reproducing the measured velocity profiles from Kipp and Grady experiments.

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PREDICTION OF DAMAGE EVOLUTION IN LAMINATED COMPOSITES SUBJECTED TO IMPACT LOADING

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Many structural components undergo significant structural damage when they are subjected to ballistic impact. Because this damage can lead to failure of monolithic components to perform their intended missions, composite structures have recently been developed to better withstand impact. The intent of these new types of composites is to provide tougher, yet lighter structures that will withstand significantly larger ballistic impact energies than do traditional monolithic structures. Although these new composite structures do indeed appear to provide increased toughness, they also undergo much more complicated damage mechanisms, so that it has become difficult to accurately predict the limits of usefulness of structures made with these materials.

It is evident that in order to develop design tools that can be used to assess the performance characteristics of these composite components, it is necessary to develop models that can accurately predict the evolution of damage of various types during actual impact events. This paper outlines a methodology based in continuum mechanics and utilizing advanced damage, fracture, and computational mechanics to obtain accurate predictions of damage evolution in laminated composite structures during ballistic impact. The evolution of damage is accounted for by the use of a cohesive zone model capable of predicting matrix, fiber, and interply cracking in ductile polymers. This model has been implemented to a global three dimensional finite element computer code for the purpose of predicting the evolution of damage during impact. The resulting algorithm is utilized herein to predict the types of damage events experimentally observed in laminated composite plates subjected to impact, and comparisons are made to two experimental results obtained by the author and co-workers.

SOME ISSUES CONCERNING THE IMPLEMENTATION OF ADVANCED CONSTITUTIVE RELATIONS IN HYDROCODES

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Materials under shock loading undergo large increases in strain, strain rate and temperature in a short space of time. In order to predictively simulate the response of these materials in this regime the constitutive model needs to account for these effects on the flow stress of the material. This implies, by definition, that the hydrocode can accurately predict the relevant strains, strain rates and temperatures as input to the constitutive model. This paper outlines potential problems and issues concerning the definition of these terms in relation to the constitutive model and their effect on the simulation result.

All the constitutive relations presently in the hydrocodes use the effective plastic strain, which is defined in terms of all the strain components including the shear strains. Material testing, however, has shown that there is a significant difference in the deformation behaviour under uniaxial conditions and torsion. In particular the work-hardening rate is much lower in torsion, but this is not accounted for within the constitutive relation. In order to describe this behaviour, the effective plastic strain within the constitutive relation must be deconvoluted into an uniaxial and shear component. This must also maintain the compatibility with the return of the stresses to the Von Mises yield surface and the subsequent calculation of the effective plastic strain. This type of relation has been implemented in the **GRIM** and **DYNA** hydrocodes and examples are shown of its consequence.

Another crucial component of the constitutive relation is the definition and calculation of temperature from the hydrocode. The most common method for calculating the temperature is based on a division of the total internal energy divided by the specific heat capacity using the hugoniot as the reference equation of state. This raises the issue of the variation of the specific heat capacity with temperature and pressure and the partitioning of the internal energy in terms of subtracting the dilational energy (ie pdv term). Other methods redefine the reference state based on cold compression curves with the inherent difficulty of experimentally determining these reference states directly. Further techniques attempt to redefine the reference state in terms of the adiabat or isotherm which raises similar issues.

Under conditions of relatively uniform deformation at medium strain rates (1 000s-1), where the temperature rises are relatively modest, the partitioning of the internal energy has little effect. However, when one considers localisation processes in deformation, including shock, then the strain rate and temperature rises are much larger and these effects become significant. The resolution of these issues may determine whether these intense localisation effects can ever be simulated predictively.

IMPLEMENTATION OF THE JOHNSON DAMAGE MODELIN THE EXPLICIT HYDROCODE OURANOUS

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in impact configuration, the damage model used until now was simple internal. To have a modelisation more realistic of the damage, it need to use more sophisticate model. Johnson's model is one of these for ductile materials. Those model is strongly non linear. There is a strong coupling between damage and the constitutive equations of the materials. So, the implementation of the need to be done carefully. To do that, a Runge-Kutta algorithm has been implemented in the Eulerian hydrocode OURANOS. Convergence conditions for the use of the algorithm are given. Unidimensional numerical test are presented with experimental results. Simulation of perforation in 2D cylindrical configuration are shown and compared to experimental results.

EQUATION OF STATE (EOS) MODELS FOR HYDROCODES

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The rapid and ongoing growth in computing power is making it possible to perform two and three-dimensional 'hydrocode" (*) simulations of many continuum shock wave applications involving large deformations and material flow, and to attack problems that would have been considered completely

impractical only few years ago. The large deformations and slow in such problems often require sophisticated numerical rezoning and/or advection procedures that cause diffusion of material EOS (#) parameters and material interfaces. Furthermore, the EOS parameters of interest include not only the classical pressure, volume, and temperature, but also the internal state strength variables that govern the evolution of plastic flow and material failure. Installation of EOS models in hydrocodes is of course very code-specific, and is typically very challenging for complex EOS models. In this paper we confine ourselves to discussing general guidelines for construction EOS models that are as "hydrocode-friendly' as possible.

We focus in this paper on three main guidelines, (1) thermodynamic respectability (obeys the second law), (2) uniqueness (well-posed and independent of cell size and other numeric features), and (3) simplicity (minimisation of model parameters that must be carried in the calculation).

We illustrate the guidelines with examples from mesomechanics.

(*) We use the term "hydrocode" to cover a large range of explicit continuum codes, including free Lagrange, Eulerian, mixed Eulerian-Lagrange, and "smooth particle hydrodynamics" (SPH).

(#) We use the term "EOS" to denote the subroutine that calculated the increment in the complete stress tensor from the increment in the complete strain tensor, i.e. the constitutive relations.

EQUATION OF STATE IN MATHEMATICAL MODELS OF CONTINUOUS MECHANICS

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The system of conservation laws for mass, momentum and energy is closed by evolutionary equations for processes taking place in a substance and equations of state (EOS) describing the materials properties in stable state. A wide range of physical states and, hence, a wide range of variation of pressure P, temperature T and other thermodynamical parameters are typical for many applied problems (managed thermonuclear fusion, development of antimeteoroid protection for space crafts, accidents in nuclear reactions, etc). EOS should describe material properties with sufficient accuracy in wide range of P, T.

A semiempirical approach for EOS construction is considered in the present work. The form of one of thermodynamical potentials is stated using a theoretical conception. The experimental data are used to determine the numerical values of coefficients in these dependencies. Such approach allows to use the experimental and calculational information and gives an opportunity to construct EOS in the compact form convenient information and gives an opportunity to construct EOS in the compact form convenient for numerical calculations. Mathematical models for the nonstationary dynamical processes impose on EOS the requirements of their effective including into computational procedure. The caloric EOS with regard to pressure P, density p, internal energy E and the thermal EOS with regard to variables P, p, T are considered. The conceptual issues of EOS constructing, the general issues concerning the totality of EOS, the particular EOS for metals, rocks, plastic materials and explosives are presented in the work. A comparison of the developed EOS with the theoretical models and the experimental data are given.

A special consideration is given for the phase transition description. On the phase boundaries many thermodynamical parameters (sonic velocity, compressibility, heat capacity, etc) are discontinue. These discontinuities are the sources of finite errors. To eliminate them one should modify the

difference conservation laws. The ways allowing to restrict the error while simulating flows with phase transition are considered.

CALCULATION OF SHOCK COMPRESSION DATA AND PHASE DIAGRAM FOR CHLORINE SUBSTITUTED METHANE COMPOUNDS

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The chlorine substituted methane compounds are of interest because of their application in the so called indicator method that allows to study high-rate processes in shock waves. In the basis of this method there are measurements of shock wave luminosity when the shock wave travelling through a studied sample enters into an indicator. As usually, a chlorine substituted methane compound is used as the indicator. A reliable interpretation of experimental data requires a full description of physical processes in the indicator and a possibility for numerical simulation of hydrodynamic flow in the experimental set up during experiment.

Here we present the physical model which describes the processes in these materials under shock loading and takes into account the experimental conditions.

The variational perturbation theory and an analogue of the Lindemann melting law namely a constancy of packing fraction along a melting curve have been applied for calculation of melting curves for some substituted methane compounds (di-chloromethane, chloroform and tetrachloromethane). The obtained results have been compared with the experimental ones. On the basis of these calculations we have made a conclusion about the nature of the methane compounds transformation under shock compression.

The equation of state for the chlorine substituted methane compounds taking dissociation into account has been constructed on the basis of the variational perturbation theory and the van der Waalse one fluid model. When comparing the calculated Hugoniots with the experimental ones it has been shown that relaxation processes may strongly affect a shape of the experimental Hugoniots. Having provided for the rate of a dissociation reaction it became possible to obtain results that rather well agree with experimental ones.

WIDE-RANGE HUGONIOTS OF POROUS SUBSTANCES

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Modern static compressions reach pressures up to 1-2 Mbar. Shock wave experiments give much higher pressures: up to 5-10 Mbar in light gas guns with plane geometry and 25 Mbar in semi-spherical explosion devices (up to 500 Mbar in underground nuclear explosions, but treatment of these measurements is complicated and less reliable).

Dynamic experiments give only Hugoniot but not the whole equation of state (EOS) of substance. At $P < 2$ Mbar it is possible to reconstruct EOS from Hugoniot with descent accuracy using models connecting cold compression curve with heat terms. At larger pressures these models have insufficient accuracy. But one *ab initio* method is known which constructs EOS from a series of Hugoniots for different initial densities.

The more we know on Hugoniots the better this method works. At P > 100 Mbar Hugoniots may be calculated by the quasi-band model with high precision; at 100-300 Mbar the quantum-statistical model gives somewhat less but good accuracy. But there is no experimental or theoretical data for the most part of substances in the gap 5-1 00 Mbars.

It occurred that experimental and theoretical parts of Hugoniots in (D - u) - variables are almost straight lines situated closely. This permits to approximate them by parabolic spline with 1~2 knots providing the same accuracy - 1% that experimental and theoretical data have. Checking with measurement in underground nuclear explosions showed that this approximation has the accuracy - 1% in the intermediate region.

This method may be applied for porous substances. Now initial parts of Hugoniots for a dozen metals and some other substances are measured up to porosity m-10. Quantumstatistical calculations for them are easily performed. Spline coefficients dependence on *m* occurred very simple everywhere except region of P < 1 Mbar. This permits to construct wide-range Hugoniots for pressures 1-100 Mbar and porosities m = 1 - 10 in the form D(u); transformation to another variables is trivial.

ALPHA TO EPSILON PHASE TRANSITION IN IRON, AND RAREFACTION SHOCKS

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Time-resolved experiments have been performed on iron to study the $\alpha \rightarrow \varepsilon$, transition. A 50 mm bore single-stage gas gun was used to accelerate projectiles with embedded single crystal Z-cut sapphire. Time resolved velocity interferometry (a VISAR) was the primary diagnostic. Experiments were designed to look for multiple wave structure on both shock compression, and release. Results of these experiments show clear evidence for the phase transition upon loading. A rarefaction shock is taken as evidence for reverse transformation on release. Analysis of the experiments was done using the CHARADE wave propagation code and results will be discussed.

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MODEL OF SOLID AND LIQUID MATTER. EQUATIONS OF STATE FOR SOLID AND LIQUID PHASES OF SUBSTANCE.

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The present equations of state of condensed matter in the solid and liquid phase give a quite satisfactory description of numerous experimental data, obtained under static and dynamic conditions in a wide range of pressures and densities. The strong shock wave compression of solid matter in the form of a fine powder offers a unique possibility of studying thermodynamic properties of condensed matter under high pressures and temperatures, but simultaneously at densities less than the normal density. Measurement of intensifies of light emitted by the shock wave front in a transparent dielectric allows to determine the temperature of the shocked material under high pressures and, hence to obtain a unique information about thermal properties of matter. In the present report it is illustrated on the example of well investigated materials which are typical for their class: copper as a metal, NaCl as a transparent ionic crystal, and liquid xenon.

These results allowed to find the type and parameters of the equation of sate (EOS) of crystal modifications and the liquid phase of this materials, including their phase diagrams. We use the Debye form of the crystalline solid EOS. The liquid phase EOS near the melting curve is quite near to the crystal EOS and at high temperatures it transforms gradually to the ideal gas EOS. In metal the electron effect manifests itself already at low temperatures in the solid phase. Analysis shows that the calculated shock adiabats of metal powders are determined in much by the electron components in EOS. In the equation of state of liquid NaCl and Xe the electron component contribution should be taken into account at temperatures beyond 10000K. We give the calculate results on the shock front structure in dielectrics determined by the kinetics of heating of electrons during their interaction with the crystal lattice. Within the scope of the model considered an explanation is given to the experimental data for a shock compressed dielectric obtained at high temperatures. Also are noted the questions requiring a further study.

THE DEVELOPMENT OF THE GENERA SUITE OF EQUATIONS OF STATE FOR ELEMENTS COVERING SOLID AND LIQUID STATES, THE MELT LOCUS, AND THE LIQUID/VAPOUR REGION

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In the absence of the capability for carrying out experiments on materials subject to very high shock pressures, with release paths involving liquid and vapour states, emphasis has increased on generating equation of state data which reflects, more closely than in the past, the physics and thermodynamics of materials under these conditions. If such improved equations of state were to be used in sophisticated hydrocodes, they would be expected to produce results more closely matching material behaviour previously observed, and give confidence in predicting behaviour when there are no such confirmatory experiments.

The Genera-S treatment for solid elements is based on a new Γ, φ, ν differential equation incorporating Gruneisen's $\Gamma(\nu)$ and its relation to potential energy ($\varphi(\nu)$, rather than on the thermodynamic $\Gamma(\nu,T)$ which derives from existing Γ, ρ, ν differential equations of various kinds. The developments have at all times maintained, as closely as possible, internal thermodynamic self consistency, and make use of experimental data to provide the baseline. From experimental data treated by Genera-S, we obtain $\Gamma(\nu)$, $\varphi(\nu)$ and their derivatives, together with E, ρ, ν, T, S over the whole field.

Genera-L uses the liquid equation of state model deriving from early work by
J Frenket and J E & M G Mayer, and treats the liquid as equilibrium states of a mixed population of free atoms and crystallises (clusters) covering a range of sizes. Using this model, together with the Genera-S results, the melt locus can be calculated by integration, to give melt temperature and pressure as functions of volume, together with latent heat and expansion on melting as well as liquidus and solidus loci.

Genera-C, based on the Extended Theory of Corresponding States and the database produced by Hougen, Watson by Ragatz, but put into analytic form, calculates, from nine pieces of experimental data, the critical point parameters, and the variation of thermodynamic parameters E, ρ, ν, T, S throughout the liquid/vapour region and along the saturation curve, including the variation of latent heat of vaporisation with temperature.

Further work is proceeding on the development of the supercritical fluid state. A database of Genera equations of state is being built.

CALCULATION OF ELECTRON PHASE PARAMETERS OF ELEMENTS AND COMPOUNDS USING COMPRESSIBILITY DATA

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The model is presented to compute energy of a compressed atom and obtain on its base the semi-empirical equation of state of solids. On the basis of this model analytical expressions were obtained for the dependences of elastic energy and elastic pressure on the compression degree which describe an experiment for many materials well. The method used allows to relate the change in energy at material compression to the equilibrium energy of outer electrons in the atomic cell of a solid and estimate the effective energy of atomic state by the known value of the bulk modulus.

The developed method allows to estimate on the base of static and dynamic experiment data the parameters of the equation of state of material in a given phase state and sometimes detect presence of various phased when it is difficult to detect this with other methods.

The analysis conducted shows that for many materials under standard conditions and, the more so, at compression features relating to various states of electrons in the atomic cell of a solid manifest themselves. From the standpoint of electron structure study of great interest are experiments both in the high pressure region and under moderate pressures where specific electron states arise providing a very valuable information about the electron structure of material and its variation under an external effect.

In many cases the model under consideration provides explanation of the complex course of material compressibility basing on the concept that different regions of P(p) or D(u) curves correspond to compression of different (including electron) phases of material. It was possible to identify the clearly nonlinear region of the D(u) dependence with compression of the phase of the material other than the initial one (i.e. having another crystal density and another bulk modulus).

Among the obtained results, the great number of various phases even for simple materials engages our attention. Their number increases with increasing pressure level. The values of energy for various phases obtained from experimental data processing may differ dramatically. It seems that the multiplicity of the electron phases of solids is a reflection of the diversity of energy of the electron excited states of atoms which is observed in the atomic spectroscopy. The difference is that in the atomic spectroscopy the energy levels of a free atom are observed, while in a solid the energy levels of a fixed-volume atom are.

THEORETICAL ANALYSIS OF THE SHOCK-INDUCED PHASE TRANSITION IN IRON

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We have studied the metastabiiity and dynamics of the shock-induced a - E: phase transition in iron. Regarding metastability, it has long been known that the experimental Hugoniot does not agree with the theoretical equilibrium Hugoniot in the two-phase region above 13 Gpa. We will present a physically based construction of the metastable phase transition surface, and will show that this surface is essentially the same in shocks as in quasistatic diamondcell experiments. Regarding dynamics, we first establish the correct irreversible thermodynamic basis for linear relaxation, then compare numerical wave propagation calculations with VISAR measurements of wave profiles. The

phase transition relaxation time is found to vary from 12-60 ns, for shocks respectively from 30-16 Gpa, and we conclude that some nonlinear relaxation must be present.

RELEVANCE OF DAC STATIC MEASUREMENTS TO MATERIALS MODELLING IN HYDROCODES

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Data for materials modelling in hydrocodes derives from a combination of shock wave experiments and static measurements. Equations of state from static experiments in DACs are now becoming available for some materials for pressures over 1 Mbar - we describe DAC experiments and review the current data. Most of this is at 300K, while theory is often extrapolated from zero K. We consider the implications of this and conclude that a cryogenic DAC facility would be valuable. We finish with a brief discussion of ideas for a cryogenic DAC capability at the Daresbury synchrotron.

USE OF Z-PINCH SOURCES FOR HIGH-PRESSURE EOS STUDIES

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There is a continuing need to measure the equation-of-state and constitutive material properties of materials to multi-megabar pressures. High-velocity launchers continue to be the standard tool for making these measurements. However, conventional gun technology is limited to launch velocities of about 8 km/s. This will produce shock pressures in materials ranging from about 7 Mbar in high-Z materials to about 1 Mbar in plastics and other low shock-impedance materials. Existing scientific and programmatic problems, however, require equation-of-state (EOS) studies to shock pressures to tens of megabars. There is, therefore, a need to increase the velocity of launchers to significantly higher velocities and to develop other sources for high-pressure EOS studies.

A variety of radiation sources are being explored for accessing the extremely high-pressure states of matter. Principal approaches being explored include lasers and pulsed power methods. Recent results obtained with laser techniques have produced promising results for high-pressure EOS studies in plastics and in deuterium. Experimental conditions, however, limit the samples sizes possible with laser sources. This results in limitations for studying a broader range of material properties other than EOS states. An example is the measurement of compressive strength in shocked states. Typically, these measurements require samples of several centimetres in diameter and several millimetres in thickness.

Pulsed power sources can be used to accelerate light ions or electrons for direct particle deposition, resulting in planar shock wave formation. Another approach is to use pulsed power methods to produce high currents in a cylindrical array of fine wires. Formation of a plasma state in the wires and implosion through the self-magnetic field produces an x radiation environment that can also produce shock waves for EOS studies. The advantage of this technique is that uniform shock wave loading can be produced on samples considerably larger than the sample sizes characteristic of laser sources.

HIGH ACCURACY EOS EXPERIMENTS USING THE AWE HELEN LASER

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A knowledge of a material's equation-of-state (EOS) is essential for hydrodynamic calculations. Although laser experiments investigate the pressure range between those attainable by gas guns (<few Mbar) and UGT's (>10Mbar) where no other data exist, it is still advantageous to obtain high accuracy data to discriminate between EOS models which have been compared with gas gun and UGT data to a few percent in pressure.

The AWE HELEN laser is being used to obtain high pressure Hugoniot data by the impedance match method. Indirect drive generates pressures up to 10Mbar in the aluminium reference material. Shock velocities are obtained by observing the visible light emitted on break-out from the surface of the target using optical streak cameras.

Experiments have been performed on copper and brominated plastic.

Attention to target fabrication and metrology, diagnostic calibration, shock uniformity and attenuation and data analysis have enabled us to measure shock velocities to an accuracy of - 1 %.

LASER-LAUNCHED MINIFLYERS FOR DYNAMIC MATERIAL PROPERTY STUDIES, AND THE ASSOCIATED OPTICAL DIAGNOSTICS

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A moderate size (10-20 Joule) laboratory laser is used to launch miniature flyer plates (2-50 micron thick by 3 mm diameter) off transparent substrates for the purpose of 1-D impact targets. The miniature flyer plate velocities can range from 0.3 to greater than 5 km/s depending on the area mass density. The flyer plates are launched with a "tophat" laser spatial profile resulting in a 1 -D plate launch and impact on the target. Because the flyer plates and targets are thin with regard to the impact velocities very high pressure gradients can be generated resulting in very high strain rates (greater than 10^7 sec-1) are easily obtained. These small, thin flyer plates require improved optical diagnostic techniques in order to quantify their performance. This is accomplished by improving the temporal resolution of VISARs (velocity interferometers) by recording the optical VISAR signals with optical fibers and streak cameras instead of PMTS. The temporal resolution is typically less than 200 picoseconds and can be less than 100 picoseconds depending on the experiment and desired resolution. We have routinely recorded and resolved shock ringing in aluminium plates 3.5 micron thick.

Thin laser-launched flyer plates have numerous applications that can probe experimental areas either not possible or extremely difficult to do with traditional gas guns and explosively-launched flyer plates. Laser-launched miniature flyer plates have been used to measure EOS and spa]] strength of metals, span strength of metallceramic interfaces where the ceramic thickness was 5 microns, and the span strength of multilayer organics where the thickness of each of four layers was typically 25 microns. Laser-launched miniflyers have the ability to experimentally quantify the dynamic behaviour near the grain size of most materials. The experimental method and data will be presented.

TIME-RESOLVED CHEMICAL CHANGES INDUCED BY PULSED LASER HEATING IN AMMONIUM PERCHLORATE AT STATIC HIGH PRESSURES

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An understanding of the chemical decomposition of energetic materials at high pressure and temperatures is essential in modelling shock wave processes in condensed media. Experimental measurements of fast chemistry at extreme pressures and temperatures, are crucial to attain this understanding. We have investigated the pulsed laser-induced decomposition of ammonium perchlorate (AP) at static high pressures using time-resolved spectroscopy. Chemical changes induced by rapid heating from a 8 ms pulsed laser operating at 514 nm, is inferred from time-resolved absorption spectroscopy. The spectroscopic measurements were carried out at a maximum temporal resolution of 1 10 nanoseconds in the 400-550 nm wavelength region, during and up to 20 microseconds after the laser pulse. Above a threshold pressure and laser fluence, the reaction initiates, observed with an absorbance increase, but does not propagate in the material. The static pressure in the material drops and cracks are observed visually. At pressures and temperature higher than a second threshold, the reaction initiates and the AP sample is consumed. The initial pressure and laser fluence correlates with the rates of change of the absorbance. Moreover, FTIR measurements from the reaction residue, were obtained and used to identify late time products of the reaction. H20, N20 and NO have already been identified. AP decomposition as a function of initial pressure and laser fluence is determined up to 5.0 GPa and up to 30 J/cm^2 respectively. The role of pressure and laser fluence in the global reaction rate of AP, inferred reaction mechanisms, and implications on current models will be addressed.

ON HOW TO MAKE THE FASTEST GUN IN THE WEST

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A new gasdynamic launcher is described, in which intact projectiles weighing at least one gram can be accelerated to mass velocities of 20 km/s. The system employs a conventional 2-stage light gas gun, with the barrel modified and filled with helium to act as a pump tube for a third stage. It is demonstrated that interstage kinetic energy efficiencies of 45% are possible and that these results can be achieved while maintaining the peak pressure applied to the projectile below 2.5.GPa. A simple analysis of this system is given, from which design parameters can be readily derived, and hydrocode calculations are presented to validate the model.

PROTON RADIOGRAPHY AT LANSCE, A NEW EXPERIMENTAL TOOL FOR DYNAMIC IMAGING

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A CODE FOR PHYSICS PACKAGE ENVIRONMENT STUDIES

T N Dey

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Analyzing high explosive response in nuclear weapons subject to a wide variety of insults requires solving equations for deformations, heat transfer and chemical reaction. A new code development project at Los Alamos is aimed at providing a comprehensive computational tool with 1 -D, 2-D and 3-D capabilities for studying non-nuclear aspects of these safety problems.

Strain rates may range from quasi-static to those associated with shock waves in these problems. Therefore, implicit and explicit solvers are being supplied. Finite element discretization includes both continuum and shell elements for low to moderate strain rate analyses. Finite volume type finite difference cells are being provided for high strain rate analyses. An important user requirement is the capability to easily add new element or cell formulations, so the code design attempts to provide a means for this while requiring only limited code modification. The underlying formulation is Lagrangian, with mesh management and mesh optimization through ALE (Arbitrary Lagrangian-Eulerian) and AMR (Adaptive MeshRefinement) techniques. Methods for correctly simulating material instability phenomena, such as shear band formation and fracture, are planned.

Heat transport can occur via conduction, convection in fluids and radiation across gaps. Contact algorithms allow impact, sliding and penetration problems to be solved.

This code is to be used for research on high explosive burn and detonation models as well as on more production oriented analyses of safety studies and experimental design. Because of this, the code uses a mixed material formulation which allows for chemical reaction and heat exchange among constituents as well as relative, interpenetrating flow. This full generality is only required under high strain rate conditions, so only subsets of this capability will be available with the lower strain rate and quasistatic solvers.

The code design has made provisions for solving the chemical reaction equations simultaneously with the equations of motion and energy to achieve better accuracy for the high explosive behaviour. This is in addition to the usual methods of solving these reaction equations within a material model with only weak coupling between this solution and the solution of the equations of motion.

DRAM - A NEW HYDROCODE OF DYNAMIC RESPONSE ANALYSIS OF MATERIAL

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The dynamic response of material under intense impulsive loading, such as fly impact, explosive, pulsed X-ray, pulsed electron beam, pulsed laser, etc, is an important subject. In order to study these questions, we wrote a hydrocode DRAM using finite difference method. In this code, there are more than ten kinds of equation-of-state (EOS), such as Mie-Gruneisen EOS, GRAY EOS, PUFF EOS, JWL EOS, etc, can be chosen by different applications. The code includes about 3000 sentences. The followings are two numerical examples performed by this code. Fig 1 is a thermal shock wave propagation in 2024 aluminium induced by pulsed X-ray, which is a lkeV blackbody spectrum with shine time of 0.05μs, and an incident fluence of 200 J/cm^2 . Fig 2 shows the propagation of a thermal shock wave in 2024 aluminium induced by an electron beam, where the

incident fluence is 200 J/cm^2, the electron energy is 0.2MeV and the irradiation time of the electron beam is 0. 12μs.

Fig 1 Thermal shock wave in 2024 Fig 2 Thermal shock wave in 2024 aluminium induced by pulsed X-ray aluminium induced by pulsed electron beam

NUMERICAL MODELLING OF NON-LINEAR WAVES DESCRIBING EQUATIONS OF HIGHER ORDER

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It is well known there are a lot of models used in Physics and Mechanics which are described by the non-linear partial differential equations of third and fourth order. As a rule such models generalise ones which are used for description of the shock wave propagation in the difference medium and keep a number of peculiarities typical for them. Examples are found in describing of long non-linear waves on a viscous fluid [1], spontaneous instabilities in premixed flames [21, non-linear saturation of the dissipate ion model by mode coupling in plasma [3] and so on.

One can point out a number of questions arisen in the numerical modelling of waves describing like models. Firstly the higher order of differential equations leads to serious restriction of mesh width in the difference equation. Secondly as a rule the non-linear models do not have any analytical solutions except for a few special solutions which it is difficult to find. Thirdly there are a number of untypical peculiarities in the non-linear waves [41.

Three models which are used in describing of non-linear waves are considered in this work. The algorithmic approach for deriving the special solutions of the non-linear partial differential equations is presented. The difference equations for numerical modelling of some non-linear waves are given. Results and peculiarities in the numerical modelling of the studied non-linear waves are discussed.

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A NEW COMPUTER CODE: DM2

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The DM2 computer code, which was originally developed as a part of a collaborative research project between NCSU and Russian Materials Center, Tomsk, uses discrete particle technique to simulate the response of monolithic, porous, or composite materials and powders under static and dynamic loading. The Russian version of DM2 is named MAC (Movable Cellular Automata) to underline its similarity to cellular automata that the materials response is simulated by movable elements that evolve in time interacting with neighbours by rules and relations.

In the DM2 materials are represented by collections of finite-sized elements that are characterized by their mechanical state (position, transitional and rotational velocities, and bonding and contact states) and thermo-chemical state (phase and composition). The motion of elements are governed by the classical equations of motion through five interactive forces: central potential force, elasto-plastic shear, viscous friction, tangential viscosity, and dry friction. Temperature change of interacting element is described by Fourier's law of heat conduction and energy dissipated from plastic and frictional interactions. Phase transition is limited to melting and solidification in which melting and freezing temperatures are specified as a function of pressure. Both stoichiometric and non-stoichlometric chemical reactions are considered in the present code. In the former, the entirety of both reacting elements are consumed during the reaction. In the latter, the reaction ceases after the limiting reagent is exhausted. The element containing the limiting reagent then becomes the product preserving the total number of elements.

This paper presents an overview of the DM2 code and some selected model calculations to show its capabilities. So far, the code has been used to simulate (1) static compression test of concrete, (2) span in single and two phase metallic alloys, (3) shock compression of HMX powder, (4) penetration of a projectile in a reactive metallic mixture, (5) chemical reactions in shear bands, (5) granular flow, and (6) particle velocity dispersion in shock-loaded heterogeneous media. A model calculation of spall in a two phase metallic alloy is illustrated in Fig 1.

Fig 1 Model calculation of spall in a two phase alloy.V_{flyer}=400m/s

MOVABLE CELLULAR AUTOMATA METHOD AS A NEW COMPUTATIONAL TECHNIQUE TO SIMULATE OF THE MATERIALS RESPONSE UNDER SHOCK LOADING

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The method of Movable Cellular Automata (MCA method) was intensively developed last years. The main ideas of the MCA method was proposed in North Carolina State University by Y Horie and S G Psakhie in 1994. In contrast to conventional net approach, the simulated medium in MCA method is

presented as an ensemble of cellular movable automata interacting among each other by some certain rules. As compared with the classic method of cellular automata, within the framework of the MCA method the medium elements (automata) are able to change not only their states but also their positions.

The evolution of the assembly of the elements is governing by the classic equations of motion, describing both translational and rotational motion. It can to noted that the MCA method allows to take into consideration the chemical reactions and phase transformations. In general case the interaction of movable cellular automaton with surrounding elements is considered as consisting of the two parts: mechanical and physico-chemical ones.

Due to mobility of each automaton the MCA method allows to take into account directly such actions as: mass mixing; penetration effects; cracks generation and development; fragmentation and fracture of materials; phase transformations and chemical reactions, etc.

It has to be noted that the MCA method comprises all the advantages of conventional cellular automata approach. This is a result of the new concept introduction:- ***"the state of the pair of automata"*** ("relation" of interacting pair of automata) in addition to the conventional one: ""**the *state of a separate automatons*** The introduction of this definition allowed to go from the net concept to the concept of neighbors. As a result of this the automata have ability to change their neighbors by switching the states ("relations") of the pairs.

Within the framework of the Movable Cellular Automata method the simulated material is considered as an ensemble of discrete elements (cellular automata), interacting by certain rules, relations and laws. Mechanical response of the ensemble of the automata is defined by "relations" of interacting pairs and the forces of inter-element interaction. Resistance of the automaton to the change of its volume is taken into account. Since in MCA method the size of an automaton is introduced directly, then for complete description of the system evolution it is necessary to add the equations for the moments to the motion equations for the mass center's. Using boundary conditions of different types it is possible to imitate different properties of surrounding medium, containing the simulated system.

Special SW was developed on base of this method and used to modelling of the high rate loading of heterogeneous materials, structures, parts as well as powder mixtures. The results of the simulations agree closely with the experimental data. The fields of MCA method application are discussed.

So, through the ability of the automata to change position the MCA approach allows vastly fill out the application fields in addition to the conventional Cellular Automata method. Due to its unique potential abilities the Movable Cellular Automata method can be considered as the solid ground for breakthrough in the computational techniques.

STIFF METHOD OF LINES FOR PROBLEMS OF CONTINUOUS MEDIA

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Problems of continuous media are usually described with system of partial derivatives equations and, perhaps, ordinary derivatives equations. Combustion of gases in nozzles or detonation may be examples; one uses gas dynamics equations for them adding chemical kinetics equations.

Such problems are traditionally calculated by the method of splitting on processes. A difference scheme is written for each equation. Values at a new time moment are calculated not simultaneously for all equations, but separately for consequent equations. When one equation (for example, impulse equation) is solved, all values from other equations (temperature, energy, concentrations of chemical components) are "frozen". Nevertheless a lot of difficulties arise. If each equation is solved by explicit scheme, the resulting algorithm is simple; but it may lose stability when the Courant condition is violated in the only space interval. Absolutely stable implicit schemes need iteration in each equation, and they not always converge. The simplest modification of the splitting method has poor accuracy, and for better accuracy one should use time consuming iterations among all equations. That is why applied codes are usually complicated rather slow and their reliability is insufficient.

We prefer an alternative approach - stiff method of lines (SMOL).

Let us change space derivatives, as usual in the method of lines. Then the problem turns into a huge system of ordinary differential equations. It is vector function consists of all physical value (velocities, densities, temperatures, concentrations of components, etc) in all knots of space grid.

This system should be solved by modern methods designed for stiff systems. Our investigation found the demands a method must suffice to provide a good numerical solution. Suitable schemes occur among Rosenbrock and Wanner schemes. They are semi-implicit and supply absolute stability. They do not need iterations and have no troubles connected with them.

Some one-dimensional tasks were calculated for checking SMOL, such as shock wave propagation and reflection from a wall, detonation wave, shock wave transformation into detonation wave and combustion transformation into detonation. The algorithm was very simple and stability took place even at enormous Courant ratios (of course far from the wave front but not near it). Possibilities of PC-286 were quite enough for these calculations.

The method is especially effective for one-dimensional problems. It provides a wide application field, because many important two- and three- dimensional problems may be approximated by one-dimensional ones with good accuracy (for example, flows of chemically reacting gases in smooth curved channels of changing cross section). The SMOL may be also successful for two-dimensional problems even on personal computers. It is perspectives for three-dimensional problems are not clear.

WAVE PROPAGATION IN LAMINATES USING THE NONHOMOGENIZED DYNAMIC METHOD OF CELLS: AN ALTERNATIVE METHOD TO STANDARD FINITE-DIFFERENCE HYDRODYNAMIC APPROACHES

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The nonhomogenized dynamic method of cells (NHDMOC) method uses a truncated expansion for the particle displacement field; the expansion parameter is the local cell position vector. In the NHDMOC method, specifying the cell structure is similar to specifying the spatial grid used in a finite-difference hydrodynamic calculation. The expansion coefficients for the particle displacement field are determined by the equation of motion, any relevant constitutive relations, plus satisfying continuity of traction and displacement at all cell boundaries.

We derive and numerically solve the NHDMOC equations for the first-, second-, and third-order expansions, appropriate for modelling a plate-impact experiment. The performance of the NHDMOC is tested, at each other, for its ability to resolve the shock wave front as it propagates through homogeneous and laminated targets. We find for both cases that the displacement field expansion converges rapidly: given the same cell widths, the first-order theory gives only a qualitative description of the propagating stress wave; the second-order theory performs much better; and the third-order theory gives small refinements over the second-order theory.

The performance of the third-order NHDMOC method, is then compared to that of a standard finite-difference hydrodynamic method. The two methods differ in that the former uses a finite-difference solution to update the time dependence of the equations, whereas the hydrodynamic calculation uses finite-difference solutions for both the temporal and spatial variables. Both theories are used to model shock-wave propagation in stainless steel arising from high-velocity planar impact. To achieve the same high quality resolution of the stress and particle velocity profiles, the NHDMOC consistently requires less fine spatial and temporal grids, and substantially less artificial viscosity to control unphysical high frequency oscillations in the numerical solutions.

Finally, the third-order NHDMOC theory is used to calculate the particle velocity for a shock wave experiment involving an epoxy-graphite laminate. Constitutive relations suitable for the various materials are used. This includes linear and nonlinear elasticity, and when appropriate, viscoelasticity. The results linear and nonlinear elasticity, and when appropriate, viscoelasticity. The results agree well with the corresponding plate-impact experiment, and are compared to the second-order theory of Clements, Johnson, and Hixson (Phys Rev E, 54, 6876 (1996)).

2-D FORMULATION OF A LINEAR MONOTONIC LIMITER FOR A 2-D LAGRANGIAN HYDRODYNAMICS WITH ARTIFICIAL VISCOSITY

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We have investigated a fully 2-d formulation of a linear monotonic limiter for a 2-d Lagrangian hydrodynamics with artificial viscosity. Rather than minmod'ing du/dx from two adjacent cells onto a node, as in 1-d, we generalize to a min-mod of the complete strain rate tensor via a number of paths that reproduce the 1-d result in the limit. We will report results on various test problems (eg Saltzmann piston problem, Coggeshall similarity solution, etc). The same methods should be applicable to displacements or strain tensors.

A GODUNOV TYPE SCHEME USING NON CONSERVATIVE VARIABLES ON LAGRANGIAN DISCRETISATION

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Many problems of mathematical physic exhibit a non conservative form equations of physic phenomena (MHD, diphasic mixture ...). A particular example occurring in continuum mechanics is the resolution of deviatoric stress tensor evolution in elastoplastic configuration. The use of conservative schemes is not possible. A new mathematical frame must be constructed to treat these problems. A conservative form of an hyperelastic formulation has been realised. It allowed to build scheme, unhappily, this is very complex. A coherent mathematical frame to take into account of non

conservative form has been built by J F Colombeau. It allows construction and justification of numerical schemes for Navier Stokes and Euler equations.

The writing of a non conservative scheme is more difficult than conservative scheme because the appropriate projection of variables must be found. Projection problem is still open for non conservative variables (plastic deformation, kinetic decomposition rate ...). We use conservative Godunov scheme as reference. Demonstration of equivalence between the Godunov scheme and our "pondere" scheme using non conservative variables is proposed. The article presents Euler equations, Riemann problem and projections in conservative and non conservative variables and their equivalence for hydrodynamic configuration.

This scheme is generalised to elastic and elastoplastic configurations. The resolution of Riemann problem is more complex than in hydrodynamic configuration (5 waves are generated). The projection with non conservative variables, as sociated to an average of deviatoric stress which is non conservative, enables to build a scheme. Results in elastic and elastoplastic tests are presented.

A TRULY PARALLEL FRAMEWORK FOR COMPUTATIONAL FLUID DYNAMICS AND COMPUTATIONAL ELECTROMAGNETICS

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To meet many present and future demands by industry in computational engineering, there is a requirement to maximise the use of high performance computers. This is particularly true in applications related to computational fluid dynamics and computational electromagnetics. To meet the challenges, the team at Swansea has been enhancing their capability of using unstructured grid methods in these application areas to operate on parallel computer platforms. The approach is truly parallel; the grid is generated in parallel which then automatically provides the domain partitions for the solvers which use message passing. The final data is output in partitioned form ready for visualisation with a parallel visualisation package. At no time is the grid and the solution data brought together since, for very large problems involving millions of tetrahedral elements, this would then create the new bottleneck. Furthermore, all the steps in the solution procedure are executed from within the Parallel Simulation User Environment (PSUE), which is a software system developed at Swansea to provide an integrated environment for application simulation, computational tools and parallel platforms.

The presentation will discuss the development of the parallel grid generator, parallel flow solver and parallel electromagnetic solver, together with an outline of the PSUE. The talk will be illustrated with examples of calculations using 10's of millions of elements.

3D ALE

T MacAbee

LLNL, Livermore, USA

HYDRA: A 3-D EULERIAN HYDROCODE

W Gaudin

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At AWE, in our 3D hydrodynamics group, our main concern is to develop computer codes for which the predominant use is safety. This often involves complicated scenarios that require a very high level of computing power to reach the required resolution. Even though we currently use some of the biggest and fastest vector machines in the world we are not hydrodynamically converged for many of our problems, and turn around times for calculations can be many hundreds of hours. With reactive burn becoming increasing important in these calculations which needs fine meshing across burn front the power and resolution needed is expanding far quicker than vector machines can cope with.

The way forward appears to be massively parallel computing which can provide the power and memory we need. However the methods for using such computers are very different from what we are used to and a good deal of thought was needed in the design. This paper details the process behind our choice for the MPP route, the code strategy, design and current results.

TECOLOTE: AN OBJECT-ORIENTED FRAMEWORK FOR HYDRODYNAMICS PHYSICS

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Tecolote is an object-oriented framework for both developing and accessing a variety of hydrodynamics models. It is written in C++, and is in turn built on another framework -- Parallel Object-Oriented Methods and Applications (POOMA). The Tecolote framework is meant to provide modules (or building blocks) to put together hydrodynamics applications that can encompass a wide variety of physics models, numerical solution options, and underlying data storage schemes, although with only those modules activated at runtime that are necessary. Tecolote has been designed to separate physics from computer science, as much as humanly possible. The POOMA framework provides fields in C++ to Tecolote that are analogous to Fortran-90-like arrays in the way that they are used, but that, in addition, have underlying load balancing, message passing, and a special scheme for compact data storage. The POOMA fields can also have unique meshes associated with them that can allow more options than just the normal regularly-spaced Cartesian mesh. They also permit one-, two-, and three-dimensions to be immediately accessible to the code developer and code user.

There are numerous advantages to having a framework in which to develop hydrodynamics methods. The most obvious is that one can build upon models (both physical and numerical) that have already been developed and tested. Also, it is advantageous for the physics programmer to have complicated computer science issues already solved, yet abstracted away. The types of computer problems that need to be solved these days, but that the physicist does not want to have to deal with, include such things as message passing and load balancing.

We have endeavoured wherever possible to write the framework in as objectoriented a manner as possible so that model developers can enjoy maximal code reuse. This has also led to a nearly complete separation of the computer science from the physics coding. The framework has also been designed to be completely portable across a wide variety of platforms.

We will discuss the philosophy of the Tecolote framework, and we will present a summary of the overall design, including a discussion of some of the objects that were used to put the framework together.

The first hydrodynamics option using the framework that we are developing is a multi-material Eulerian code. This will allow us to compare with an existing hydrocode written in Fortran 90. We will present comparisons of both timings for large problems, and of possible maximum size of problem on the computer platforms of interest at Los Alamos.

PARALLELIZATION TECHNIQUE AND HYDROCODE FOR NUMERICAL SIMULATIONS OF 3D FLOWS WITH HEAT CONDUCTIVITY

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The numerical solution of 3-D problems requires extreme computer resources represented by massively parallel distributed-memory computer systems. A successful employment of the great potential power of these systems to solve a single problem is possible only when the application software taking into account the parallel data processing is developed.

The report presents the results of the development of parallelization technique for 3-D gas dynamics problems with heat conductivity. The basic method for numerical solution of 3-D implicit finite-difference equation systems is the method of splitting by directions. The method of splitting by directions allows to reduce a complex multi-dimensional problem to a set of simpler problems and this set can be successfully realized on the parallel processors. Two basically different techniques for the massively parallel computations are developed. The first technique uses the 3-D data matrix decomposition reconstructed at the timestep and is an extension of the algorithms of parallelization for shared main memory multi-processor computer systems. The second technique is based on using the 3-D data matrix decomposition which is not reconstructed within the timestep.

The developed techniques were realized in the form of the parallel program (hydrocode) for the massively parallel distributed-memory computer systems.

The computation series were runned for the numerical study of the relative parallelization performance for various methods of geometrical problem decomposition and for two modes of processor loading. The influence of the ration (arithmetic/communication operations) on the performance was analysed also.

The quantitative estimations of the paralielization performance for the developed techniques obtained on the MP-3 and Meiko-CS2 computer systems are presented.

ARCHITECTURE OF MULTI-COMPUTER COMMUTATION NETWORK AND COMPUTATIONAL PHYSICS PROBLEMS DIFFERENCE GRID

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One of the main reserves to enhance computer system performance is massive computation parallelisation where one large problem is simultaneously computed on a great number of processor elements.

Apparently, the parallelisation performance depends on the parallelisation capability of the algorithm used, as well as on the architecture features of the multi-processor computer system employed.

The presentation discusses the algorithms for solution of evolutionary problems of computational physics discretised over r-dimensional matrix architecture difference grids and peculiarities of implementation of these algorithms on multi-processor computer systems having the matrix or hypercube architecture commutation network.

In particular, it is shown that at the matrix architecture of the commutation network a loss of mean load of the processor elements when there are quite numerous is inevitable.. The hypercubic architecture commutation network is superior regarding this parameter to the matrix architecture commutation network. Some theoretical estimations were verified by solution of the test problems on several types of the multi-processor super-computers.

A CODE DEVELOPMENT VIEW TOWARDS THE NEXT CENTURY

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As we go towards the next century, code developers need to have a vision of what their codes will be capable of and also what their users will require of their codes.

This vision and progress will have several constituents ranging from new and improved algorithms, improved physics and material models together with enhancements to the existing Massively Parallel Computers. The paper will discuss the authors view of recent future trends in the industry.

AN AUTOMATIC-REZONE CAPABILITY FOR CTH ON MASSIVELY PARALLEL COMPUTER PLATFORMS*

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The existing single-processor version of the automatic-rezone option for CTH calculations has been extended to operate on massively parallel computer platforms. The automatic-rezone option periodically rezones the computational mesh coordinates. Cell variables from the old coordinates are remapped into the new coordinates one coordinate at a time (after completion of the remap step using the same ordering scheme as the remap step). In single-processor operation, all variables in the mesh are available to the processor so it is a relatively simple matter to rezone the information from one set of coordinates into another using a combined mesh (coordinates made up of the union of old and new coordinates). In multiprocessor operation only the variables within the range of the local coordinates are available to a given processor. In this case only those new coordinates within the range of the local old coordinates are considered. The variables are remapped from the old coordinates into this sub-set of new coordinates (again using a combined mesh made up of the local old coordinates and the sub-set of global new coordinates). An additional step is then needed to transfer information from the old processor space (already remapped into new cell sizes) to the new processor that is now responsible for this particular range of coordinates.

This option is useful for simulations which occupy a small volume initially, but occupy a large volume late in the calculation (such as buried burst simulations) or simulations that require a moving mesh.

The modifications required to extend this capability from single-processor to multiprocessor platforms will be described and example calculations using this scheme will be presented.

* Computation Predictability as applied to Penetration Mechanics

ARTIFICIAL VISCOSITIES FOR 2D LAGRANGIAN CODE

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Following the successful implementation of a tensor artificial viscosity in the two-dimensional hydrocode, CORVUS a monotonic version has been developed in order to combine the best features of both methods. This paper describes the theory and implementation of the original tensor viscosity and the ideas involved in extending this to a monotonic version.

Results obtained using this artificial viscosity are shown for a number of problems, in particular the spherical Noh problem. Comparisons are made between the original tensor artificial viscosity and the monotonic version and other approaches

DESIGN OF AN EULERIAN REZONER FOR THE THREE DIMENSIONAL HYDROCODE NUTMEG

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NUTMEG is a three dimensional Eulerian hydrocode with material interface tracking and is based on the ideas formulated by Youngs. For several years NUTMEG has been successfully applied to three dimensional hydrodynamic simulations at Aldermaston. However, for certain classes of problems where the physical region of interest decreases with time - for example an imploding shell - the computational mesh becomes inefficiently used. For these types of problem it would be advantageous to rezone - focus the mesh - on the region of interest. This paper deals with the description of a 3D Eulerian rezoner. Results are then presented for two preliminary test calculations which show that the rezoner is functioning correctly and producing good accuracy.

GODUNOV'S METHOD FOR CALCULATION OF ELASTIC-PLASTIC DEFORMATION ACCOMPANYING BY PHYSICAL-CHEMICAL CONVERSIONS

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The finite-difference method of S K Godunov is now one of more popular numerical method of continuous mediums mechanics. It has been favourably for solution of gas-dynamics problems from 1959, with some gas-dynamics problems had been for the first time solved by application of just this method.

In this work, the generalization of Godunov's method has been suggested to problems of solid body dynamics and to application to simulate of high-velocity processes into deformable solids with regard to physical-chemical conversions and fracture.

The equations of thermal-elastic-plastic medium including the conservation laws and governed correlations are the base for examined mathematical model. In this model, the plastic deformation is the variant of current theory of Prandti-Reuss, the thermal effects are described by non classic (hyperbolic) thermal conductivity equation including heat inertia.

It is necessary often to take into account the optional effects accompanying the deformation: polymorfic phase transitions, solid-phase chemical reactions and fracture. In this case, the mathematical model is added by corresponding kinetic equations. The constructed equation's system of hyperbolic type is written in normal form (in resolved relatively to time-derivative form), that allows at the numerical integrating to use the ideas and principles inherent in gas-dynamics scheme of Godunov S K.

The finite-difference equations system is presented for this medium model; the automodel solution of Rieman problem is received for linear approximation; the question of correct formulation of boundary conditions is examined. As a result the time-difference scheme is received, that is analogy by internal characteristics for gasdynamics Godunov's scheme. It is explicit homogeneous monotonous divergent scheme of first order accuracy. The convenience of increase of approximation order to second one at the retaining of monotony of scheme is discussed in this work.

The comparison of analytical and numerical solutions is conducted with help of simple model problems on the propagation of longitudinal and lateral elastic waves, elastic-plastic and heat waves in half-space, that give the possibility to make conclusion that suggested finite-difference scheme reproduces sufficiently well the wave picture current from weak elastic waves to powerful shock waves described by gas-dynamics theory. However the advantages and adaptability of Godunov's scheme are exhibited more plainly at the solution of non-one-dimensional problems.

The presented here examples of two-dimensional computations on high-rate impact of cylindrical particle and metal target illustrate some method opportunities of employment of mobile adapting meshs to the simulation of elastic-plastic currents with large shear strains.

THE STRUCTURE OF SHOCK EJECTA FROM THE FREE SURFACE OF LEAD PLATES

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This paper describes the results of investigations into the nature of material ejected from the free surface of a lead plate by explosively driven shock waves. This ejecta is modelled in a Lagrangian hydrocode as a cloud of particles that is tracked through the mesh. This cloud interacts with the surrounding air, principally though the action of drag. The effect of an increased air pressure on the particulate cloud is to slow down the leading ejecta and shorten the piezoprobe record, an effect that varies with the mean length scale associated with the particles. A chi-squared distribution is assumed for the masses of individual particles, based on models of diesel sprays. The code calculations are compared with the results of experiments that utilize both piezoprobe and Fabry Perot diagnostic techniques. The effect of the surface finish of the plate on the mass and velocity of ejecta is also considered.

AN AUGMENTED LAGRANGIAN FORMULATION FOR DYNAMIC CONTACT/IMPACT PROBLEMS IN AN EXPLICIT LAGRANGIAN FINITE ELEMENT CODE

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In a lagrangian code, the mesh follows materials in this deformation. Each material is separately modelised. An algorithm is needed to take into account the interaction between them. At each time step, it gives the boundary conditions, along the contact surface, for the resolution of the differential equations system which describes the physic. This study includes friction.

In finite element discretisation, the contact conditions appear as non linear boundary conditions which are solved with an algorithm of "contact-impact". The most of them try to avoid the interpenetration of the meshes in resolving more or less the "condition of continuity" on the normal velocity along the sliding surface. One can find in the literature algorithms based on a minimization principle. But the iterative algorithm are not often used in dynamic explicit codes, where the friction is neglected.

The problem of contact can be considered as the resolution of energy minimisation under constraints principle. The most classical and rigorous methods (lagrange multiplier method, augmented lagrangian method) take iteratively into account all phenomena which are present in the contact physic process: friction, impenetrability condition and thermodynamic state of the cells connected to the slide line. The penalty method is an approximation of the minimisation problem without introduction of the new variable. It is easy to implement but the limit conditions are not correctly treated.

Our choice involves an augmented lagrangian method associated with an Uzawa's algorithm for the resolution of the iterative system, as one can find in Simo and Laursen's works. Inside it, the equations for friction are discretised with a backward euler's scheme. The sliding limit and the sliding or stickiness states are found with the "trial state return mapping" method. This work has been developed in an general frame for dynamic phenomena and implemented in an explicit dynamic lagrangian finite element code OURANOS.

The algorithm built up takes into account of the thermodynamical state of the cell and of the gap function. So the state of the matter is updated in function of the applied repulsion force. The solution is built iteratively by the determination of the nodes effectively in contact, of the repulsion forces and the approximation of the thermodynamic state of the cells connected to the sliding surface. The method of convergence is sure but slow. Specific lists of nodes of the sliding surfaces have been introduced, they must be up date at each iteration. The organisation of this algorithm allows to implement complex mechanical behaviour.

1 D, 2D and 3D tests are shown. The first of them, for which analytical solutions are known, allows the validation of the algorithm. The others, associated with different friction coefficients, generate softer sliding surfaces.

THE USE OF DYNA3D TO EXAMINE STRUCTURAL RESPONSE TOSHOCK LOADS IN AIR AND WATER

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This paper covers the use of the DYNA3D finite element code to examine the response of two different structures to shock loads.

Firstly, the paper describes a study which predicted the response of a masonry building to an internal explosion. To achieve this a discrete element technique was developed to enable DYNA3D to be used to model failure mechanisms of masonry structures. The technique was used to examine the response of the building to various charges in order to identify the charge mass required to demolish the building. Subsequent trials with actual buildings, subjected to blasts from the same charge masses, confirmed the model predictions. The overall damage to the building, failure patterns in the masonry and the charge size required to demolish the building were all as predicted.

The second study involved the use of DYNA3D to predict damage to a civilian ship from a mine explosion. The paper initially describes the use of DYNA3D to predict the propagation of the pressure wave and expansion of the bubble of explosion products in the water. A validation of the DYNA3D predictions with a numerical solution of gas bubble equations is shown. The work conducted to examine the response of a section of the ship's structure is then described. It is noted that the results of such analyses must be carefully interpreted to account for the variation in material behaviour at the high strain rates which occur under shock loading.

The work outlined in the paper illustrates the capability of DYNA3D (with some modifications) to model the response of various structures to shock loads.

MULTI-DIMENSIONAL UPWINDING FOR THE EULER EQUATIONS

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COMPUTER MODELLING OF "SHOCK-INDUCED" AND "SHOCK-ASSISTED" CHEMICAL REACTIONS IN POWDER MIXTURES

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The experimental investigations of reactions of synthesis in powder mixtures under shock loading have revealed the existence of two kinds of chemical processes. These processes were named "shock-induced' and 'shock-assisted". Specific character of these chemical processes is not well studied till now.

New model of mechano-chemical processes in two-component porous mixtures under shock-wave loading is proposed in this work. The model is used to investigate the synthesis of new solid phases in such powder mixtures as NI-AI, TI-AI, TI-SI, Ti-C under plane shock wave loading. The main aim

of the modelling was to study the degree of chemical conversion in powder mixtures with different initial porosity and concentration of the components at the shock pressures in the range of 100-200 kbar.

The model of mechano-chemical processes includes three groups of equations. The first group consists of equations of mechanical conservation laws and laws of phenomenological thermodynamics. The second group includes the equations of state for multiphase medium. Kinetic equations of creation of new chemical phases and densification of porous medium are united in the third group.

Chemical kinetics of solid phase reactions is closely connected with the physical mechanisms of mass transfer and mechanisms of plastic deformation. Thus, the kinetic equations are different for "shock-induced" and "shock-assisted" chemical reactions. If the mass transfer especially connected with the plastic flow of solid components, the reaction will take place in the front of shock waves. Thus, the "shock-induced" chemical reaction is finished behind the shock wave front. The "shock-assisted" chemical reaction is not stopped behind the front due to creation of the liquid phase.

The chemical reaction of synthesis produces the energy release and heats the reaction products. The energy release accelerates the chemical conversions and transforms the structure of the shock wave front. The "shock-induced" chemical reaction lead to acceleration of the shock wave front propagation and to some certain rise of the pressure. The chemical conversion is not complete in the stoichiometric powder mixture after shock wave loading with the amplitudes of 100 Kbar. The reduction of a duration of a shock pulse reduces the degree of chemical conversions.

PROPAGATION OF WEAK SHOCK WAVES IN SHELLS OF REVOLUTION

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As a practice in today's separation technology for space launchers vehicles, pyrotechnical devices are widely used. Thus, during separation of rocket stages or payload, shock waves appear, which must be studied to give proof for structural resistance with respect to induced stresses and acceleration levels. For this purpose an efficient algorithms has been constructed. The numerical method and results from its application to some dedicated examples, will be presented.

The method uses a mixed nodal and Fourier-discretization. Fourier-discretization transforms the partial shell differential equation into an ordinary one, which is solved subsequently exactly by numerical integration over the rotational axis parameter x. As a result, finite shell elements of revolution are generated for each Fourier-coefficient, which are used to build and to solve a mathematical model differential equation of second order in time.

In order to obtain a sufficient good representation of the wave front from the solution, a small nodal mesh - within the unit of the shell thickness - is necessary. This, however, leads to a considerable large number of shell elements to be generated and degrees of freedom to be used for the solution. Therefore a number of high efficient methods are introduced to save numerical effort. First, a sparse matrix technique arising from the rotational symmetry, second a high-order Runge-Kutta method for time and spatial integration and not at least a new recursive method for the generation of exact shell elements has turned out to process very accurate solutions within hour of PC computational time, even for large systems.

SIMULATION OF DYNAMIC PROCESSES IN CONDENSED MATTER ON UNSTRUCTURED MESHES

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Godunov and derived high order methods are widely applied in aerodynamics for solution of hyperbolic system of conservation laws. Results achieved caused to implementation of this approach for solution of problems of condensed matter dynamics, where we have to take into account both smooth and discontinuous flows. Godunov-type methods are to based on closed system of conservation laws in divergent form. Conservation laws for mass, momentum and energy are well known, but equation for symmetric deformation tensor are principally could not be written in divergent form. Therefore law of conservation of velocity and deformation fields compatibility replaces this equation. This equation uses nonsymmetric tensor of deformation gradient. Conservation laws are closed by constitutive equations. such as a wide range semiempirical equation of state and kinetic equations for damage and nonelastic deformations growth. This approach correspond to elastic-viscoplastic model (kinematic hardening) and connected with impossibility of full divergent form for elastoplastic model.

Riemann problem is solved on the base of parabolic approximation of shock Hugoniot. Various types of boundary conditions are simply specified by solution of Riemann problem between boundary cell and ghost cell with appropriate parameters. Method is realized on nonstructured near-Lagrangian grid.

Grid points move with Lagrangian velocities. Since we use Delaunay triangulation at every time layer, conservation laws are integrated over Dirichiet cell.

Computer code developed is applied for simulation of hypervelocity impact, motion of cosmic bodies in planet atmosphere, beams interaction with condensed target. These computations show high flexibility of approach and ability of solution of problems with strong shock and rarefaction waves, large deformations and phase transitions.

CORVUS 3D

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A 3D Arbitrary Lagrangian Eulerian (ALE) hydrocode is under development at AWE. The intention is to extend the algorithms used in AWE's 2D ALE code CORVUS where possible. The Lagrangian part of the algorithm has been generalised and implemented in a prototype code. This employs explicitly integrated, trilinear isoparametric finite elements for the spatial discretisation and a predictor-corrector time step with one intermediate stage.

A prototype code has been produced and is being used to validate the algorithm and to assess a range of important issues before work on the production code commences. In particular, the data structure chosen and the amount of data that is stored rather than being recalculated is crucial to obtaining a balance between memory requirements and run time. In addition it must be determined whether the explicit integration as used in CORVUS is practical in 3D or whether numerical integration must be used.

These issues are of vital importance as the code is intended to be used for large memory, long run time, 3D simulations, and must run efficiently on both the MPP architecture of an IBM SP2 and vector architecture of a CRAY C98D. Ultimately a range of physics packages and numerical techniques such as ALE and AMR will be added to the code, so it is important to devise a data structure that will not restrict the efficiency with which these packages can be implemented and coupled to the code.

The conclusions that have been made to date regarding the above issues along with the results of some idealised test problems will be presented.

USING LOCAL RECONSTRUCTIONS OF THE IRREGULAR LAGRANGIAN GRID AT COMPUTING MULTI-DIMENSIONAL GAS DYNAMICS PROBLEMS WITH LARGE DEFORMATIONS

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The Lagrangian method is an extraordinarily powerful technique for solving gas dynamical problems. However, its drawback is that when computing flows with large material deformations the grid distortion takes place which can lead to timestep reduction and sometimes to impossibility of computation continuation without a preliminary grid reconstruction.

The Lagrangian grid reconstruction was widely used mainly in the 2D hydrocodes and, besides, as applied to regular (quadrangular) grids.

Recently the interest has quickened in various unstructured and irregular grids which are much more readily reconstructable and, in addition, allow to localise the grid areas subjected to reconstructions.

Thus, this presentation is devoted to consideration of the issues of development of the technique for local reconstructions of 3D (and 2D) grids whose cells are represented by Voronov bodies (and arbitrary convex polygons) at the initial time and by arbitrary polyhedral during the subsequent grid deformation and reconstruction. The focus is therewith made on the aspects of reconstruction of the grid geometry and architectural connections.

The local operations of the grid reconstruction are based on two principal operations: paste of two cells having a common face and cut of one cell into two ones by some plane. Introduction of just these two operations is accounted for by the following considerations:

(1) both the operations meet the principal grid reconstruction requirements, that is allow to refine or coarsen the grid when needed;

(2) the cell cut and paste operations do not change the grid topological structure:

(3) being the elementary operations on grid cells, these operations can be used as blocks for reconstruction of other, more complex operation of grid reconstruction.

At local reconstructions all problem integral characteristics are preserved which positively tells on accuracy of the computation conducted.

The presentation pays attention to the issue of development of the criteria for local grid reconstructions. The performance of the proposed method is demonstrated with the results of two model computations.

DMK HYDROCODE FOR SOLVING CONTINUUM MECHANICS PROBLEMS

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The DMK hydrocode is designed for a computation of the 2-D time-dependent continuum mechanics problems taking into account the material strength properties, the heat conductivity and motion of the disperse phase particles on the background of the carrying medium motion. The hydrocode includes the techniques based on the regular and irregular difference grids which can be used simultaneously in various regions of the problem solved.

The solution technique is Lagrangian one and the difference scheme is the generalised Neumann scheme. The grid composed of convex polygons connected to and moving with material is used for the irregular computational grid.

Using the irregular grid considerably simplifies its construction because it permits to apply the arbitrary polygons in an arbitrary order. The irregular grids allow to introduce the procedure of the local grid reconstruction by means of cutting the separate cell or pasting the two neighbouring cells. This not only simplifies the solution of the problems with the large materials deformation, but also allows to compute the problems with varying topology of the computational regions. The grid secures the cell convexity.

The DMK hydrocode technique is based on the following principles:

(1) splitting the problem computed into the computational regions;
(2) simultaneous use of regular or irregular grid technique in each computational region;
(3) splitting by physical processes;
(4) computation with the separated interfaces.

The automatic determination of the neighbouring computational regions is realized in the DMK hydrocode.

The DMK hydrocode is developed in the FORTRAN language and is composed of three parts.'

(1) computation of the initial grid and the gas dynamical parameters defined on this grid.,
(2) computation of the timestep of the continuum mechanics equation integration;
(3) visualization of the results.

The specialized language for the initial geometry description is used for the preparation of the initial grid.

Both sequential and parallel versions of the DMK hydrocode are developed.

The report presents some examples of numerical simulations.

PENETRATION ANALYSES

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Penetration analyses have traditionally been fertile ground for studying problems in which computation and experiment overlap. Within the testable regime, computations have been used to

analyze experiments and tests and synthesize the information gathered from multiple tests. In many cases, this type of computation allows us to interpolate among experiments and achieve a more unified understanding of the phenomena under study than we would otherwise gain from experimentation alone. We are typically confident in our ability to do this because important issues can still be directly addressed by experiments. Thus, we are usually not in a position where a critical question must be answered solely by a calculation.

In the case of impact studies, when impact velocities increase beyond the testable regime, we can no longer perform controlled experiments. They are either impossible physically or too expensive to perform. In this regime, computation has historically assumed a different role, which we prefer to call exploratory. The intent of this computational approach is to extrapolate beyond existing experimental data. But, little firm reliance is placed upon such extrapolations when real systems are under construction, nor is it clear that it should it be. One is often confronted with the rather bizarre situation that very detailed computations are performed which are not ultimately trusted.

None the less, there is increasing need to extrapolate beyond the testable regime using simulations. This is because, for a variety of reasons, we are making the transition from a test-dominated to simulation-dominated development cycle for many applications. the fundamental scientific question that must then be answered in order to accomplish this transition is the following: How accurate are the simulation predictions beyond the testable regime? However, the authors take a broader view and claim that a somewhat different question must be answered: What quantitative techniques are required to establish an adequate level of trust in simulation predictions beyond the testable regime?

One field which has devoted considerable attention to this problem is computational fluid dynamics (CFD). This has been fuelled by the search for the 'Holy Grail" of CFD - the development of a "Computational Wind Tunnel' that would replace, in many respects, actual wind tunnel testing in the design of aerodynamic bodies. Whether or not such a computational capability already exists is a moot point. Currently, the operational approach is to use a judicious blend of experiment and computation, with the experiment the preferred means of resolving critical issues.

Similar work seems to be lacking in the field of penetration mechanics, although a variety of needed pieces exits. The purpose of our paper is to discuss issues, approaches, and problems that are involved in performing this work. A guiding principle that we have found relevant is: "Everything becomes hard when one seeks predictability beyond the testable regime." We will thus focus our discussion on the problems of establishing trust in software predictability. We will also state our view that, for complex simulations, establishing trust in their predictability requires the language and techniques of statistical inference. To illustrate this latter point, we will summarize statistical experimental design techniques that can be used to quantify computational sensitivities when dealing with uncertainty in complex simulations.

REACTIVE HYDROCODE SIMULATIONS OF SHOCK-TO-DETONATION PHENOMENA IN GRANULAR HMX AND COMPOSITE PBX

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Conventional explosives remain a foundation of modern military defense systems. However, spurious detonations due to low velocity impacts and their often tragic consequences highlight our lack of understanding of the microstructure/chemistry linkage. The suspension of reactive crystals in a viscoplastic binder to form plastic bonded explosives (PBXS) is often employed to produce energetic composites with more precisely controlled sensitivity than binderless aggregates. This

practice tends to reduce the performance of the composite from that of monolithic aggregate. Therefore, it is of interest to optimize the geometric and material properties of PBXs so that the greatest degree of control can be maintained over the sensitivity with a minimal degradation in performance. The current study simulates the shock induced formation of localized heating in both binderiess and composite microstructures of HMX (ie PBX9501) employing a 2D Eulerian finite element hydrocode. Real micrographs of energetic material are image processed and imported into the finite element mesh directly, giving the capacity for predicting localized heating in relevant geometries with realistic particle size distributions of tens or hundreds of particles of high explosive (HE). Relevant physical processes including melting with temperature, pressure and rate dependent flow stress, latent heat of fusion effects during phase transitions, heat conduction and simple multistep chemical reaction with gas have been implemented into the hydrocode. Initially, a comparison was made between the hot spot distribution due to intergranular and intragranular voids in the binderless explosive. It was determined that the hot-spot volume and peak temperatures due to collapse of intragranular voids are similar to those predicted at the particle interfaces due to collapse of intergranular voids. The same calculations were performed for a cast PBX containing intragranular voids only. It was determined that the binder absorbs a large fraction of the shock energy through bulk heating. However, the binder also tends to increase the peak temperatures predicted near collapsing intragranular voids. Binder properties of density, specific heat and yield strength were varied. It was determined that, for negligible porosity, HE crystal temperatures are predicted to be essentially insensitive to binder strength and heat capacity. Additional, it was observed that binder densities below that of the HE give minimal predicted heating of the crystals. This result contradicts conventional wisdom which presumes that minimal HE heating will occur for impedance matched binder and HE. Preliminary reactive calculations for the porous aggregate demonstrate good agreement with experimental observations of run-to-detonation vs shock pressure (Pop plots). Permeation of hot gaseous products into the porous bed ahead of the shock induced reaction zone is captured and is demonstrated to be an important mechanism in the shock-to-detonation process.

THE USE OF DETONATION MODELS IN UNDERSTANDING DETONATION PHYSICS

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Traditionally detonation models were created as a means of allowing the performance of explosives to be accurately modelled in metal forming applications and in blast dynamics. Most models were aimed at reproducing the energy release rate of ideal explosives. In some cases these models were extended to include non-ideal effects such as finite reaction time, or initiation behaviour.

More detailed modelling approaches included terms for the intrinsic reactivity of the explosive, and for the geometry of the reaction front as it progressed from ignition sites through the bulk explosive. The modus operandi was to parameterise the model from data and then use the model to predict explosive performance in the geometry of interest under various initial and boundary conditions. The accuracy of the model in representing the detonation process was not of primary concern as the calibration data was never far from that being simulated. The results of the model per se were not regarded as independently significant outwith the required simulations. In this work an alternative approach is taken, where the detonation model is used a means of probing the detonation physics occurring in non-ideal detonation in powder explosives.

The small divergent flow detonation code, CPeX, is reviewed and the kinetic model examined. The model is fitted to published charge diameter effect data for various powder explosives, generating sets of kinetic parameters. The variation of predicted reaction rates and reaction co-ordinates

through the reaction zone is mapped. The kinetic model is used to construct isobaric reaction profiles for the various explosives, from which the effect of particle size and intrinsic reactivity on the detonation kinetics is investigated. In particular the relation of the reaction rate function to "Group 1 and Group 2" behaviour is reviewed.

From the results of the model it is found that reaction tends to be of the hot spot and grain burning type at low density but of progressively more thermal explosion type at higher densities. Small particle size results in an increase in the tendency to thermal explosion as does an increase in the intrinsic reactivity at any particle size. The results can be understood in terms of the interaction of the shock wave with the porous structure, the number and size of the resultant hot spots, the distance between hot spots and the inherent chemical reactivity of the explosive.

Finally it is shown that the use of detonation models to understand detonation physics can be extended to other types of methods, more specifically to the "ignition and growth" class of equations.

PSC IMPLEMENTATIONS OF THE WBL MODEL

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The WBL model supplies equations of motion and boundary conditions governing the propagation of the leading shock of a detonation wave. The model is based on two assumptions

> the detonation speed D is a function of local wave curvature K the angle a detonation wave makes at an inert boundary is constrained by a value or range

Initial implementations of the model used wave-tracking to predict detonation propagation, i.e. approximating the wave as a finite set of Lagrangian marker particles propagating according to the WBL equations of motion.

Recent implementations have adopted a fundamentally different approach, using the "Propagation of Surfaces under Curvature" (PSC) method - also known as level set methods. These schemes calculate wave propagation by relating it to a selected isosurface embedded in an evolving field defined throughout the problem. This method is particularly suited to problems with multiple wave collisions and complicated boundary interactions.

The first generation of such schemes were restricted to calculating problems defined on a cartesian mesh. A second generation has since been written in which the scheme's algorithms have been generalised to allow the calculation of 2D and 3D arbitrary mesh problems.

DETONATION WAVE FRONT STRUCTURE OF CONDENSED HIGH EXPLOSIVE

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The interferometer systems: Fabry - Perot and ORVIS for investigation fine structure of detonation of detonation front of solid high explosive with nanosecond time resolution are used. To register mass velocity U window method is used. Crystals Li F, water and other materials are used as the window. Thin foil (aluminum 6-20 micrometer) was place between the window and the explosive.

For different high explosives different mass velocity profiles in the reaction zone are registered. In the mixture high explosive on PETN basis, when the detonation wave reaches explosive -window threshold the condition of P=32GPa, U=1,65 km/c must be realised. We fixed the condition U=2,1 km/c, that corresponds to P+45 Gpa, which felled during 7 ns up to Jouget point U=1,6 km/c.

We received some results on registration of front detonation structure in the reaction zone for other high explosives (TNT, RDX, HMX and other).

In the report we explain the experimental results and make the attempt to build the new detonation model.

SHOCK-WAVE INITIATION OF POROUS ENERGETIC MATERIALS AND VISCO-PLASTIC MODEL OF HOT SPOTS

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General trends in the behaviour of the shock-to-detonation process in condensed heterogeneous explosives, including the nonmonotonic dependence of explosive material specific surface on shock sensitivity, are reviewed. A strong correlation between the critical detonation diameter d_{cr} and initial specific surface A_s of heterogeneous condensed individual explosives is show to exist (d_{cr} A_s Const at a constant EM density).

A modified one-dimensional visco-plastic model of hot spot formation in shock pressurized energetic materials is formulated. For the case of temperature-independent visco-plastic properties of inert materials an accurate analytical solution is derived in the limit of small Reynolds numbers which describes hot spot formation during pore deformation caused by both shock waves of different duration and ramp waves with different pressurization rates. The effect of heat conduction on hot spot formation is analyzed. The estimated critical pore size below which formation of hot spots is suppressed by heat conduction is in good agreement with experiment. Indirect estimates of the viscosity reported by various researchers for some energetic materials are discussed.

The reasonable agreement of this model with most of the experimental data demonstrates that for a wide class of energetic materials, namely, for pressed and cast explosives, the hot-spot model must take into account visco-plastic properties of energetic materials.

AN APPROXIMATE BUT COMPLETE SIMULATION OF REACTION IN HETEROGENEOUS EXPLOSIVES

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The geometrical aspects of chemical reaction in heterogeneous explosives was modelled by direct simulation of random assemblies of reactive particles. A packing algorithm was used to fill a volume with particles of varying but predetermined type and diameter, such that the resultant configuration was representative of a multi-phase multi-component explosive. The array of particles was mapped onto a logically regular three dimensional grid that was subsequently collapsed unidirectionally, forcing voids (gas filled particles) to form cusps. Solid particles were sheared by the flow. Material in the deformed grid was consumed using a simple Huygens wave principle to mimic flame propagation

from the cusps. Each component reacted at a constant predetermined rate, and no secondary reaction between the various reaction products was allowed. A computational grid of 64 x 64 x 128 was used with periodic boundary conditions, giving an assembly of between 103 and 104 particles per simulation.

Simulations were performed on a three component system: voids, liquid matrix and solid particles. The mean diameter ratio of bubbles to solid particles was varied from 10:1 to 1:10. The ratio of combustion velocity between liquid and solid was also varied from 10:1 to 1:10. The phase volume ratio of the bubbles to solids was held close to 1: the phase volume of the liquid, not an independent variable, was always found to be close to 0.4.

The effect of geometrical factors on the reaction rate of heterogeneous systems was demonstrated. Fastest reaction was found for mixtures of equally sized solids and voids with the liquid and solid reaction rate equal. Percolation effects were noted for mixtures containing small highly reactive solids, when the flame front was carried by the solid phase.

EXPERIMENTAL EVIDENCE LINKING IMPACT AND SHOCK INITIATION

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Recent experiments have demonstrated that the small scale Ballistic Impact Chamber (BIC) Test can rank the relative shock initiation sensitivity of explosives. The data base for this is now quite large, extending over several thousands of tests. The agreement between the BIC test results and known large scale initiation sensitivity tests is extremely good.

This represents a very interesting development not only because of its potential usefulness, but also because shock and impact initiation processes have never been linked and are normally though of as unrelated. A brief description of the BIC test will be given along with a description of our understanding why these impact test results rank relative shock sensitivity. (A more complete description will be given in the associated paper submitted by CSC.) A portion of the BIC and relative shock sensitivity results will also be presented. This will include not only several standard HMX and RDX based explosives but also some ammonium nitrate/fuel oil compositions. In summary, the data shows that it should be possible to analytically treat initiation by shock or impact on an equal footing.

SHOCK INDUCED DETONATION-LIKE REACTIONS IN METAL/TEFLON SYSTEMS

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A study of shock induced reactions in a metal/teflon mixture was undertaken. One-Dimensional plane wave embedded gauge and wedge test experiments have demonstrated that a self-supported detonation-like wave is induced into these materials. The shock induced reactions revealed a chemical reaction build-up similar to A1/oxidiser energetic materials! Specifically most of the reactions occurred at the shock front. The wedge test data revealed the characteristics associated with a steady state detonation reaction wave. Namely, near constant reaction propagation velocity and pressure. An empirical ignition and growth model containing global kinetics for the detonation-like state and for the slower metal reactions subsequent to this state has been applied to these results and will be presented!!

CAPABILITY'S AND DEFICIENCY'S SIMULATION'S ON NUMERICAL SIMULATIONS TO TAKE INTO ACCOUNT THE PHYSIC OF MECHANISMS ON TERMINAL BALLISTIC

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The contribution of numerical simulations to the understanding of the mechanisms gives today to the numerical tool a main role for the future's preparation in the field of military heads and armours. That is why CEG has been used for many years numerical simulations in complement of detonics experimentations. The numerical works presented here are performed with the OURANOS 2D Eulerian version hydrocode. Equations of continuum mechanics are solved with a finite differences scheme. Interface tracking in mixed cells is solved with Youngs and SLIC algorithms. Following geometries are studied:

penetration of a ceramic armour (AL23 Alumina or SIC) by a tungsten alloy rod in a DOP configuration.

penetration in or perforation of a steel armour (XC48 or Mars 190) by a XC48 steel EFP.

For metals, the equation of state is a Murnaghan type EOS. They are modelized with the Zerilli-Armstrong or Johnson-Cook constitutive models and a Von Mises equivalent stress. The damage of ceramic materials (compression/tension) is taken into account by the Johnson-Holmquist model. The parameters of this model have been identified or evaluated from the results of our set laboratory experiments (Plate-impact, SHPB and Pyrotechnical Divergent Spherical experiments).

By the knowledge of the materials behaviour, simulations allowed a good restitution of the experimental results. The correlation between experimental results and numerical simulations in this case is quite acceptable.

If the penetration aspect seems to be numerically reproducible, some problems related to the perforation process remains, due to the damage/rupture mechanisms which are not yet physically and numerically controlled. For instance, a shear banding appears in the case of perforation limit.

MODELLING OF SHEAR BANDS IN MESOVOLUMES OF METALS UNDER SHOCK LOADING AND UNLOADING

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The purpose of the work is numerical investigation of the process of deformation localisation in mesovolumes of metals under dynamic loading. The approach is based on mesomechanics. The mesovolumes of metal materials represent a set of grains of different orientation from several up to hundreds grains. In the later case this mesovolume may be considered as representative, over which it is possible to carry out averaging. Such volume forms macro-particle of a material in usual understanding in mechanics of continuous media. Significant elements of mesostructure of material are obviously taken into account in mesovolumes: 1) orientation of grains, each grain has its individual yield strength; 2) boundaries of grains; 3) if necessary, near boundaries areas are prescribed separately, for which the resistance to elastic-plastic deformation can differ from average resistance to shear deformation in grain; 4) various hard inclusions (segregations) are prescribed.

So any local areas, their configuration are specified obviously, for which physical mechanical characteristics differ from environmental material. For numerical investigations the finite-difference scheme in Lagrangian variables known as Wilkins method was applied.

Results of our investigation show that in such heterogeneous medium under dynamic loading the plastic deformation is developed as especially local process. The plastic shears generate in the areas of stress concentration and are developed in kind of bands of localised shear. The sizes of such bands is determined by many factors, basic of which are the power of stress concentrator and development of hardening or loss of strength in the region of formed shears. So from joints of grains, hard particles, with sizes less or commensurable with sizes of grain, shear bands of rather small capacity are developed, which pass through one or some grains or along boundaries of grains, if the boundaries have lesser strength than shear strength of grains themselves. More powerful stress concentrators and larger scale heterogeneities create areas of strain localisation which can cover on width some grains and to pass through several grains.

It is shown that system of localised shear bands break material into separate blocks which at further deformation move and rotate as units. The deformation of blocks has mainly accommodation character and is necessary for preservation of material continuity. These blocks are possible to consider as structural elements of deformation of mesoscopic scale.

The all-round compression which is realised in shock wave essentially changes character of shear bands development. In this case the bands of localised shear are formed mainly by initial structural heterogeneities of mesoscopic scales: grains, hard inclusions. The rotations of separate elements of mesostructure are well defined. Set of bands is oriented in direction of maximum tangential stresses with their inclination about 4511 to the shock front. Characteristic length of shear bands is

approximately equal to the size of appropriate structural heterogeneities. In release waves the deformation increases just in shear bands formed in shock front.

Thus, advanced approach permits to investigate numerically peculiarities of plastic deformation of materials with consideration for their real structural heterogeneity. It has allowed for the first time to model process of formation and development of shear bands in an explicit form and so to describe a stage of prefracture of material.

DATABASE FOR PROPERTIES OF MATERIALS STUDIED IN EXPERIMENT USING SHOCK WAVES

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During nearly 50-year period of development of the dynamic methods for studying material properties Russia accumulated a large amount of experimental data for more than 200 individual materials, compounds, condensed media and gases. Practically all the information is obtained at RFNC-VNIIEF. For the accumulated experimental data systemisation and visualisation the database being presented was developed. At its development DBMS Paradox for Windows was used. The databases is a set on interconnected tables storing:

* the data for shock compression of continuous materials
* the data for shock compression of heated materials
* the data for shock compression of porous materials
* the data for shock compression of materials by the second shock wave

* expansion adiabats of shock-compressed continuous materials
* expansion adiabats of shock-compressed porous materials
* the data for the rate of scattering of shock-compressed
* materials to air
* the data for sound speed in shock-compressed materials

Currently the database stores the data for the following material types: metals; metal hydrides and nitrides; carbides and oxides; mixtures; solid organic materials; alkali metal halogenides; minerals and rocks; water and saturated water solutions of salts; organic liquids.

As the data is (and will be) transferred to the Experimental data base from a great number of various sources (papers and reports), it also stores the complete list of these sources.

SPALL MODELLING IN HYDRODYNAMICS

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Further refinements to our implementation of the Johnson void growth model in 2D hydrocodes are described. A consistent treatment of temperature effects is now included and a treatment of failure when voids coalesce has been developed. The temperature dependence of span strength in the model is tested by comparison with the results of a series of plate impact experiments on aluminium with varying initial temperatures. Observations of spallation in experiments carried out using the AWE HELEN laser also compare favourably with the model predictions. The short pulse durations typical in the latter experiments enable data to be obtained on the strain rate dependence of spall strength which provide a more stringent test of the model's capabilities.

A MODEL FOR ESTIMATION OF METAL TEMPERATURE BEHIND SHOCK WAVE FRONT

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The model accounts potential nucleus-electron interaction, nuclei thermal motion, thermal electron excitation. Nuclei thermal capacity is described by a function which secures smooth transition from solid heat capacity to ideal single atom gas heat capacity. At low temperatures electron gas is considered as degenerate, electron heat capacity is proportional to temperature. Electron gas degeneracy removal with temperature is taken into account. When temperature is much higher than Ferni temperature, electron gas is considered ideal. The paper gives description of the algorithm. It uses analytical dependencies. To compute temperature by the suggested model, the following must be set: density, Grueneisen factor, material bond energy under standard conditions, the parameters of shock wave front dependence on mass velocity behind the front, the value of initial material density for which this dependence has been obtained. The computed results are compared with experimental data for copper and computations using other models for copper, molybdenum and aluminium.

INVESTIGATION OF STRESS RELAXATION AT MICRO- AND MESOSCALE LEVELS IN MATERIAL MESOVOLUMES UNDER SHOCK WAVE LOADING

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Stress relax processes in heterogeneous materials and investigated. The stress relaxation in materials is attributed to development of shears caused by both dislocation motion and formation of shear bands commensurable With sizes of structural fragments (for example, grains) on the mesoscale level. These mechanisms are of different physical nature and cause fast relax processes (in shock wave fronts) and slow ones (in macro volumes of material).

Relax constitutive equations are constructed where deformation is described as both evolution of dislocation continuum on the micro level and development of plastic strain localisation on the mesolevel.
Under weak shock waves the heterogeneous nucleation of dislocations occurs even in elastic precursor (an initial dislocation density cannot provide the experimental observed rate of elastic precursor decay). Defect generation processes begin to play an essential role in shock wave fronts, when the plastic deformation has developed. The experimental profiles show that unloading is of viscous elastic nature and cannot be described in terms of elastic-plastic theories. In the model the processes are taken into account.

There is a great number of dislocations of various types behind a shock wave front. For instance, the tendency of deformation to organise itself in dislocation patterns is observed. Various stress magnitudes are necessary for them to be started. To account for the feature, the function of defect distribution has been incorporated into the model formulation. This allows one to fit the calculated and experimental observed release wave profiles.

To take into account the non-ideal Bauschinger effect a reversible plastic deformation, which allows for unfastening dislocations, when a sign of loading changes, is introduced into the model.

For simulation of strong shock waves a homogeneous defect nucleation, which play a main role in formation of the strong wave front structure, is incorporated into the consideration.

In material mesovolumes the average yield strength is connected with mesosubstructure formation and shear band evolution. The processes are taken into account by introducing characteristic times of relaxation into the model to construct the phenomenological constitutive equation.

The process of loading of mesovolume is simulated and the relax times are derived. Calculations are carried out at the macro level. The constitutive equations using the relax times are applied.

MD INVESTIGATION OF DISLOCATION INTERACTION IN FCC METALS

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LANL, Los Alamos, USA

EQUATION OF STATE AND WAVE PROFILES IN SHOCKED FOAMS

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Gas gun shock impact experiments have been carried out on several foams which had initial densities of 0.3 g/cm^3. Materials included a polyurethane foam with a large cell structure (up to mm size voids) and foams with microballoons to create the voids. Particle-velocity wave profiles were measured using magnetic particle velocity gauges on each side of the foam and using VISAR interferometry on the downstream side of the foam. Samples were 5 and 7 *mm* thick with a PMMA window on the back so that the crushed-up foams were reshocked as the wave reflected from the PMMA. Inputs to the foam were 0.3 GPa and above. Preliminary equation of state models have been developed based on Hermann P-a formalism.

AB FERE INITIO EQUATIONS OF STATE FOR ALUMINIUM AND SILICON

D Swift

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Finding electron ground states using the local density approximation, and adding quasiharmonic phonon states, ab initio equations of state have been calculated for aluminium and silicon. The equilibrium density is a few percent too large.

If the equation of state is forced to match the equilibrium density by adding a pressure offset, the resulting ab fere initio equation of state is brought into much closer agreement with experimental shock wave data.

COMPARISON OF WILLIAMSBURG WITH JWL EQUATION OF STATE FOR NITROMETHANE

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The Williamsburg is a thermodynamically consistent equation of state for detonation products. The Williamsburg parameters were fitted to chemical equilibrium calculations for nitromethane. The resulting equation of state is compared with the tabular equation to which it was fitted, and with a JWL equation of state fitted to experimental data. The performance of the equations of state is evaluated in hydrocode calculations of a cylinder test.

DIRAC ELECTRON STATES IN CONDENSED MATTER

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A scheme is under development for finding electron states in condensed matter by minimising the Dirac Hamiltonian to enable spin and relativistic effects to be incorporated. At present, the scheme represents electrons as a single quantum field, using the local density approximation to include the

effects of exchange and correlation. All integrations are performed in real space, which makes it simple to allow arbitrary basis functions.

SHOCK COMPRESSION OF HIGHLY POROUS SAMPLES OF COPPER, IRON, NICKEL AND THEIR EQUATION OF STATE

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Shock compressibility to -90 GPa is studied for samples of copper, iron and nickel of initial density 5-20 times as low as normal. The porous samples are obtained from fine-grain powder of several hundreds (2-£ of angstrom in size of individual grains. For shock loading explosive generators were used which create planar and spherical shock waves in samples. In the experiments the shock wave velocity in porous samples was recorded. At pressures higher than 1 0 Gpa wire electric contact sensors were used and at lower pressures when operation of these sensors is not sufficiently stable the measurements were taken with piezoelectric sensors. The obtained data is compared with computations by the equation of the state of metals at a variable heat capacity of nuclei and electrons.

WIDE-RANGE HUGONIOTS OF POROUS SUBSTANCES

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Modern static compressions reach pressures up to 1-2 Mbar. Shock wave experiments give much higher pressures: up to 5-1 0 Mbar in light gas guns with plane geometry and 25 Mbar in semi-spherical explosion devices (up to 500 Mbar in underground nuclear explosions, but treatment of these measurements is complicated and less reliable).

Dynamic experiments give only Hugoniot but not the whole equation of state (EOS) of substance. At $P < 2$ Mbar it is possible to reconstruct EOS from Hugoniot with descent accuracy using models connecting cold compression curve with heat terms. At larger pressures these models have insufficient accuracy. But one *ab initio* method is known which constructs EOS from a series of Hugoniots for different initial densities.

The more we know on Hugoniots the better this method works. At $P > 1$ 00 Mbar Hugoniots may be calculated by the quasi-band model with high precision; at 100-300 Mbar the quantum-statistical model gives somewhat less but good accuracy. But there is no experimental or theoretical data for the most part of substances in the gap 5-100 Mbars.

It occurred that experimental and theoretical parts of Hugoniots in (D - u) - variables are almost straight lines situated closely. This permits to approximate them by parabolic spline with 1-2 knots providing the same accuracy - 1% that experimental and theoretical data have. Checking with measurement in underground nuclear explosions showed that this approximation has the accuracy - 1 % in the intermediate region.

This method may be applied for porous substances. Now initial parts of Hugoniots for a dozen metals and some other substances are measured up to porosity m-10. Quantum-statistical calculations for them are easily performed. Spline coefficients dependence on m occurred very

simple everywhere except region of P < 1 Mbar. This permits to construct wide-range Hugoniots for pressures 1-100 Mbar and porosities m = 1 - 10 in the form D(u); transformation to another variables is trivial.

EFFECT OF REINFORCEMENT STRUCTURE OF ORIENTED FIBREGLASS PLASTICS ON THE STRENGTH OF CIRCULAR CYLINDRICAL SHELLS DURING EXPLOSIVE INNER LOADING

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A specific load-carrying capacity of circular cylindrical fibreglass plastic shells of the same geometry has been experimentally studied during explosive inner loading. The shells have an inside diameter of 300 mm, a length of 600 mm and 8% ratio of the thickness to radius.

The reinforcement structure winding and the reinforcing element, VMPS filament and RVMN roving fibres of 0.01 mm diameter, varied. The combined reinforcement with alternating spiral and circular layers of equal thickness showed a 1.5-2 time higher load-carrying capacity than the uniform spiral layers or circular layers, irrespective of the filament type. Also the reinforcement structure predetermines the basic characteristics of dynamic reaction, mechanism and type of destruction. Authors revealed peculiarities of destruction of composite shells differ in the structure of reinforcement at different conditions of explosive loading.

The obtained experimental data were used for development of destruction model of composites, having complicated structure, at explosive loading.

CALCULATION METHOD AND MODEL OF DEFORMATION OF CERAMIC COMPOSITE WITH ALLOWANCE FOR RELAXATION, ACCUMULATION OF MICRODAMAGES AND FRACTURE

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In this work a methods of calculation of elastic-plastic deformation and fracture of elements of a structurally inhomogeneous medium on meso and macroscale under dynamic and quasi-static loading are developed. The microstructural peculiarities of a medium are taken into account within the framework of relax models, which is applied to study the influence of dislocation kinetics of plastic shears on deformation and strength properties of elementary volume of material (microdescription level). On meso and macrolevel the response of structurally inhomogeneous medium to loading is described on basis of elastic-ideally-plastic model of medium, plastic-brittle model offered by A Dragon and Z Mroz, but also variant of couple of stress model based on the concept of sliding. Plastic-brittle model of a composite takes into account mechanisms of strain hardening and loss of strength of material in accordance with accumulation of micro an mesodamages inside and on the interfaces of structural elements.

Simulation of processes of strain localisation and the development of stress concentrators of mesoscate is carried out in two dimension dynamic and quasi-static formulations. In dynamic formulation the problem is solved by a finite difference method for complete system of equations of continuous medium mechanics, recorded in divergence form for wide range of loading rates. In particular, calculations with the purpose of reception of quasi-static approach by this method are

carried out. The method is developed for description of meso and macrocracks generation on the basis of algorithm of calculation grid splitting.

On the other hand, the solution of the problem in quasi-static formulation is carried out on the basis of the Lagrange variation principle formulated for medium with nonsymmetrical stress tensor. Such formulation is necessary for expansion of application area of the method on the problems of mechanics of couple stress media. On this basis the variational difference scheme for two dimensional and three dimensional elastic-plastic problems for heterogeneous media with explicit account of internal structure heterogeneity is constructed.

The heterogeneity of mesostructure of a composite in presented two dimensional calculations is taken into account obviously as a heterogeneity of the elastic characteristics, parameters describing strain hardening and loss of strength of material at the stage of plastic flow, and also strength inside and on interfaces of bulk elements of composite structure.

Numerical modelling of effects of localisation of deformations, development of concentrators of stresses in mesovolumes of a ceramic composite, but also generation and development a meso and macrocracks is carried out. Comparison of results of calculation in quasi-static and dynamic formulation under small rates of loading is performed to test the methods.

For output on macrodescription level of a composite averaged stress-strain diagram for macrovolume of material with various internal structure are constructed.

LATE ABSTRACTS

DYNAMIC BEHAVIOUR OF PURE ALUMINAS SUBMITTED TO DIVERGENT SPHERICAL SHOCK WAVE

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The goal of this communication is to model the mechanisms (plasticity, pore closure or microcracking) generated by the propagation of a divergent spherical shock wave and their time evolutions. The studied materials are two pure aluminas, AL23 and T299, with different average grain sizes. The Pyrotechnical Spherical Divergent (PSD) experiments are used to characterise the behaviour of these aluminas.

A phenomenological analysis performed from the available experimental data is the foundation of the theoretical choices made in modelling. A Gurson-type plasticity model takes into account the effects of the pore closure on the material response. The influence of the pores and cracks presence on the elastic behaviour is considered through a homogenisation technique.

Comparatively to previous papers, several improvements are proposed for the representation and the evolution of the damaged states due to microcracking. In particular, a damage criterion in extension is introduced.

Numerical calculations performed with a Wondy-type code gives satisfactory experiments - calculations comparison and permit the discussion of the role of each phenomenon.

PROTON RADIOGRAPHY: A NEW TECHNIQUE FOR DYNAMIC IMAGING

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We have used the 800 MeV proton beam at the Los Alamos Neutron Science Center (LANSCE) to obtain time-resolved images of the propagating burn front in a small high explosive assembly. The assembly consists of a 30 cm diameter charge of LX07, an HMX-based high explosive, surrounded by a 13 cm thick hemispherical shell of PBX 9502, TATB-based high explosive. We have imaged the burn front at 4 times referenced to detonator breakout: 0.99 msec, 1.90 msec, 2.50 msec, and 3.25 msec. In all cases a very nearly spherical burn front is observed. Behind the burn front, and consistent with the statistical precision of our measurements, we see a density distribution which is characteristic of the reaction zone followed by the adiabatic expansion of the product gases. In the later time measurements we clearly see the boundary between the LX07 and PBX9502 explosion products.

I will discuss the theoretical background for our imaging technique, including the use of magnet lenses to remove the unavoidable blurring in the image plane due to multiple-coulomb scattering (MCS) in the object; experimental details; the data; and our analysis of the data to date. I will also discuss the static experiments we have performed on a nested-shell spherical object in a 10 GeV/c proton beam line at the Brookhaven National Laboratory (BNL) Alternating Gradient Synchroton (AGS).

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